# FIGURE 3

#### **LEGEND**

Column headings from left to right are (A) 'Atom Number', (B) 'Atom Type', (C) 'Amino Acid', (D) 'Chain Identifier', (E) 'Amino Acid Number', (F) 'X Coordinate', (G) 'Y Coordinate', (H) 'Z Coordinate', (I) 'Occupancy' (OCC) and (J) 'B factor'.

А	В	С	D	E		F	G	Н	I	J
1	N	ALA	Α	126	-1	.225	18.275	58.94	19 1.00	62.30
2	CA	ALA				).160	18.687	59.90		
3	СВ	ALA				351	20.162	60.31		
4	С	ALA				.137	17.763	61.12		
5	0	ALA	Α	126	-(	.940	17.908	62.04	14 1.00	61.53
6	N	ALA	Α	127		.784	16.805	61.12		
7	CA	ALA			(	.859	15.815	62.17		
8	СВ	ALA	Α	127	1	.255	14.482	61.59	99 1.00	57.77
9	С	ALA	Α	127	1	.878	16.247	63.20	05 1.00	56.23
10	0	ALA	Α	127	3	3.075	16.075	63.00	00 1.00	56.65
11	N	TRP	Α	128	1	.401	16.816	64.30	1.00	53.28
12	CA	TRP	Α	128	2	2.263	17.245	65.38	30 1.00	50.98
13	СВ	TRP	Α	128	1	.566	18.369	66.13	33 1.00	51.50
14	CG	TRP	Α	128	1	.402	19.546	65.26	58 1.00	52.38
15	CD1	TRP	Α	128		.246	20.024	64.71	1.00	53.18
16	NE1	TRP	Α	128	(	.515	21.153	63.97		
17	CE2	TRP		128		.862	21.394	64.01	1.00	
18	CD2	TRP	Α	128		2.442	20.405	64.83		
19	CE3	TRP	Α	128		3.820	20.440	65.04		
20	CZ3	TRP		128		1.554	21.416	64.45		53.73
21	CH2			128		3.949	22.391	63.66		
22	CZ2			128		2.606	22.395	63.43		
23	С	TRP		128		2.517	16.093	66.33		
24	0	TRP		128		.747	15.154	66.37		
25	N	ALA		129		3.598	16.200	67.10		
26	CA	ALA				3.992	15.236	68.11		
27	СВ	ALA				.028	14.287	67.55		
28	С	ALA				1.596	16.072	69.26		
29	0	ALA				1.980	17.220	69.03		
30	N	LEU				1.659	15.530	70.48		
31	CA	LEU		130		5.155	16.302	71.62		
32	CB	LEU		130		5.119	15.469	72.90		
33	CG	LEU				1.612	16.028	74.26		
34	CD1	LEU	A	130		5.469	15.546	75.41		
35	CD2			130		1.470	17.523	74.31		
36	С	LEU		130		5.570	16.796	71.34		
37	O N	LEU	A	130 131		5.933 7.349	17.927 15.967	71.72		
38 39	N CA	GLU GLU		131		3.736		70.65		
39 40	CA CB	GLU		131		3.736 3.506	16.309 15.118	69.66		
41	CG	GLU	A			).077	14.915	68.21		
42	CD	GLU				3.560	13.599	67.61		
72	CD	GTO	Д	тот	3		10.000	07.01	1.00	JJ.04

## FIGURE 3<u>A</u>-(Cont.)

A	В	С	D	E	F	G	Н	I	J
43	OE1	GLU	Α	131	8.836	13.078	66.726	1.00	64.32
44	OE2	GLU	Α	131	10.648	13.084	67.993	1.00	63.67
45	С	GLU		131	8.937	17.577	69.485	1.00	41.74
46	0	GLU		131	10.041	18.101	69.415	1.00	41.77
47	N	ASP	А	132	7.881	18.078	68.841	1.00	39.05
48	CA	ASP	A	132	8.010	19.323	68.100	1.00	38.32
49	СВ	ASP	Α	132	6.935	19.466	67.028	1.00	39.96
50	CG	ASP	Α	132	6.946	18.299	66.066	1.00	41.30
51	OD1	ASP	A	132	8.056	17.837	65.689	1.00	46.10
52	OD2	ASP	A	132	5.894	17.772	65.723	1.00	42.94
53 54	C 0	ASP ASP	A	132	7.926	20.559	68.989	1.00	37.33
55	N	PHE	A	132 133	8.094 7.692	21.640 20.370	68.472 70.289	1.00	36.39 36.67
56	CA	PHE	A	133	7.485	21.498	71.213	1.00	37.49
57	CB	PHE	A	133	5.998	21.569	71.740	1.00	36.30
58	CG	PHE	A	133	4.958	21.474	70.656	1.00	38.62
59	CD1	PHE	A	133	4.504	22.602	69.999	1.00	38.46
60	CE1	PHE	Α	133	3.564	22.499	68.993	1.00	41.24
61	CZ	PHE	A	133	3.108	21.250	68.611	1.00	39.81
62	CE2	PHE		133	3.564	20.125	69.246	1.00	38.63
63	CD2	PHE		133	4.495	20.235	70.252	1.00	39.61
64	С	PHE	Α	133	8.475	21.593	72.399	1.00	38.04
65	0	PHE	Α	133	8.934	20.578	72.922	1.00	37.77
66	N	GLU	Α	134	8.825	22.817	72.801	1.00	37.74
67	CA	GLU		134	9.511	22.989	74.079	1.00	38.18
68	СВ	GLU	Α	134	10.583	24.031	73.989	1.00	38.70
69	CG	GLU	Α	134	11.692	23.627	73.052	1.00	45.76
70	CD	GLU		134	12.863	24.551	73.142	1.00	52.60
71	OE1	GLU		134	14.009	24.040	72.996	1.00	57.17
72	OE2	GLU		134	12.635	25.768	73.380	1.00	57.77
73	С	GLU	A	134	8.424	23.456	74.979	1.00	37.78
74	0	GLU	A	134	7.697	24.400	74.647	1.00	37.67
75 76	N	ILE		135	8.295	22.825	76.123	1.00	35.90
76 77	CA CB	ILE ILE	A A	135 135	7.223 6.657	23.145 21.878	76.998 77.499	1.00	37.06 37.79
78	CG1	ILE	A	135	5.960	21.157	76.334	1.00	41.64
79	CD1			135	4.794	20.341	76.792	1.00	48.55
80	CG2			135	5.700	22.126	78.593	1.00	37.59
81	C			135	7.682	24.058	78.152	1.00	36.78
82	0			135	8.778	23.906	78.672	1.00	34.54
83	N			136	6.819	24.998	78.533	1.00	37.69
84	CA			136	7.179	25.975	79.541	1.00	36.95
85	С			136	6.383	25.807	80.792	1.00	37.86
86	0			136	6.052	24.706	81.139	1.00	38.85
87	N	ARG		137	6.052	26.917	81.449	1.00	38.75
88	CA	ARG	Α	137	5.311	26.886	82.699	1.00	39.01
89	СВ	ARG	Α	137	5.392	28.252	83.369	1.00	40.79
90	CG			137	4.941	29.390	82.494	1.00	39.62
91	CD			137	4.835	30.762	83.163	1.00	45.72
92	NE	ARG	Α	137	3.554	30.754	83.754	1.00	48.61

# FIGURE 3

#### **LEGEND**

Column headings from left to right are (A) 'Atom Number', (B) 'Atom Type', (C) 'Amino Acid', (D) 'Chain Identifier', (E) 'Amino Acid Number', (F) 'X Coordinate', (G) 'Y Coordinate', (H) 'Z Coordinate', (I) 'Occupancy' (OCC) and (J) 'B factor'.

A	В	С	D	E	F	G	Н	I	J
1	N	ALA	Α	126	-1.225	18.275	58.949	1.00	62.30
2	CA	ALA	Α	126	-0.160	18.687	59.906	1.00	61.70
3	СВ	ALA	Α	126	-0.351	20.162	60.315	1.00	62.19
4	С	ALA	Α	126	-0.137	17.763	61.129	1.00	60.66
5	0	ALA	Α	126	-0.940	17.908	62.044	1.00	61.53
6	N	ALA	Α	127	0.784	16.805	61.123	1.00	59.08
7	CA	ALA	Α	127	0.859	15.815	62.173	1.00	57.38
8	СВ	ALA	Α	127	1.255	14.482	61.599	1.00	57.77
9	С	ALA	Α	127	1.878	16.247	63.205	1.00	56.23
10	0	ALA	Α	127	3.075	16.075	63.000	1.00	56.65
11	N	TRP	Α	128	1.401	16.816	64.301	1.00	53.28
12	CA	TRP	Α	128	2.263	17.245	65.380	1.00	50.98
13	СВ	TRP	Α	128	1.566	18.369	66.133	1.00	51.50
14	CG	TRP	Α	128	1.402		65.268	1.00	52.38
15	CD1	TRP	Α	128	0.246		64.714	1.00	53.18
16	NE1		Α	128	0.515		63.973	1.00	53.05
17	CE2			128	1.862	21.394	64.017	1.00	54.15
18	CD2	TRP	Α	128	2.442		64.834	1.00	53.19
19	CE3	TRP	Α	128	3.820		65.049	1.00	54.16
20	CZ3	TRP	Α	128	4.554		64.458	1.00	53.73
21	CH2	TRP	Α	128	3.949		63.660	1.00	54.15
22	CZ2	TRP	Α		2.606		63.431	1.00	54.51
23	С	TRP	Α	128	2.517		66.332	1.00	49.09
24	0	TRP	Α	128	1.747		66.370	1.00	48.80
25	N	ALA		129	3.598		67.100	1.00	47.28
26	CA	ALA			3.992		68.114	1.00	46.51
27	СВ	ALA		129	5.028		67.555	1.00	45.67
28	С	ALA	Α	129	4.596		69.262	1.00	45.56
29	0	ALA		129	4.980		69.037	1.00	43.83
30	N			130	4.659		70.480	1.00	46.03
31	CA	LEU	Α	130	5.155		71.628	1.00	46.26
32	СВ	LEU	Α	130	5.119		72.909	1.00	46.46
33	CG		Α	130	4.612		74.261	1.00	49.12
34	CD1	LEU	Α	130	5.469		75.419	1.00	47.91
35	CD2		Α	130	4.470		74.311	1.00	46.43
36	С	LEU		130	6.570		71.348	1.00	46.06
37	0	LEU	A	130	6.933		71.722	1.00	45.86
38	N	GLU	Α	131	7.349		70.657	1.00	44.57
39	CA		A	131	8.736		70.328	1.00	43.80
40	СВ	GLU	A	131	9.506		69.669	1.00	45.34
41	CG	GLU	A	131	9.077		68.219	1.00	50.12
42	CD	GLU	Α	131	9.560	13.599	67.616	1.00	59.64

#### FIGURE 3A

A	В	С	D	E	F	G	Н	I	J
43	OE1	GLU	Α	131	8.836	13.078	66.726	1.00	64.32
44	OE2	GLU	Α	131	10.648	13.084	67.993		63.67
45	С	GLU	Α	131	8.937	17.577	69.485	1.00	41.74
46	0	GLU	Α	131	10.041	18.101	69.415	1.00	41.77
47	N	ASP		132	7.881	18.078	68.841	1.00	39.05
48	CA		Α		8.010	19.323	68.100	1.00	38.32
49	СВ	ASP	Α	132	6.935	19.466	67.028	1.00	39.96
50	CG	ASP	А	132	6.946	18.299	66.066	1.00	41.30
51	OD1	ASP	Α	132	8.056	17.837	65.689	1.00	46.10
52	OD2	ASP		132	5.894	17.772	65.723		42.94
53 54	С		A	132	7.926	20.559	68.989	1.00	37.33
54 55	O N	ASP			8.094	21.640 20.370	68.472 70.289	1.00	36.39
56	CA		A A		7.692 7.485	21.498	70.269	1.00	36.67 37.49
57	CB		A		5.998	21.4569	71.740	1.00	
58	CG	PHE			4.958	21.474	70.656		38.62
59	CD1	PHE	Α	133	4.504	22.602	69.999	1.00	38.46
60	CE1		A	133	3.564	22.499	68.993	1.00	41.24
61	CZ	PHE	Α	133	3.108	21.250	68.611	1.00	39.81
62	CE2	PHE	Α	133	3.564	20.125	69.246	1.00	38.63
63	CD2	PHE	Α	133	4.495	20.235	70.252	1.00	39.61
64	С	PHE	Α	133	8.475	21.593	72.399	1.00	38.04
65	0	PHE	А		8.934	20.578	72.922	1.00	37.77
66	N	GLU		134	8.825	22.817	72.801	1.00	37.74
67	CA	GLU		134	9.511	22.989	74.079	1.00	38.18
68	СВ	GLU		134	10.583	24.031	73.989	1.00	38.70
69	CG	GLU		134	11.692	23.627	73.052		45.76
70	CD OF 1	GLU		134	12.863	24.551	73.142	1.00	52.60
71 72	OE1 OE2	GLU		134 134	14.009 12.635	24.040 25.768	72.996 73.380	1.00	57.17 57.77
73	C	GLU GLU		134	8.424	23.456	74.979	1.00	37.78
74	0			134	7.697	24.400	74.647	1.00	37.67
75	N			135	8.295	22.825	76.123		35.90
76	CA		Α	135	7.223	23.145	76.998		37.06
77	СВ	ILE	A	135	6.657	21.878	77.499	1.00	37.79
78	CG1	ILE	Α	135	5.960	21.157	76.334	1.00	41.64
79	CD1	ILE	Α	135	4.794	20.341	76.792	1.00	48.55
80	CG2	ILE	Α	135	5.700	22.126		1.00	37.59
81	С	ILE	Α	135	7.682	24.058	78.152		36.78
82	0	ILE	Α	135	8.778	23.906	78.672		34.54
83	N			136	6.819	24.998	78.533		37.69
84	CA			136	7.179	25.975	79.541		36.95
85	С			136	6.383	25.807	80.792		37.86
86	0	GLY			6.052	24.706	81.139	1.00	38.85
87	N C7	ARG		137	6.052	26.917	81.449	1.00	38.75
88 89	CA CB	ARG ARG		137 137	5.311 5.392	26.886 28.252	82.699 83.369	1.00	39.01 40.79
90	CG			137	4.941	29.390	82.494		39.62
91	CD			137	4.835	30.762	83.163		45.72
92	NE			137	3.554	30.754	83.754		48.61
		_		-	<del>-</del>				

## FIGURE 3B

A	В	С	D	E	F	G	Н	I	J
93	CZ	ARG	Α	137	2.501	31.519	83.484	1.00	42.31
94	NH1	ARG			2.481	32.576	82.674	1.00	39.40
95	NH2	ARG			1.423	31.205	84.148	1.00	40.08
96	С	ARG			3.841	26.591	82.437	1.00	38.31
97	0	ARG			3.319	26.884	81.363	1.00	35.25
98	N	PRO			3.186	26.035	83.432	1.00	38.59
99	CA	PRO			1.741	25.812	83.367	1.00	37.99
100	CB	PRO			1.416	25.119	84.688	1.00	38.79
101	CG	PRO			2.691	24.697	85.283	1.00	38.62
102	CD			138	3.782	25.569	84.712	1.00	
103	СЪ	PRO			1.059	27.163	83.333	1.00	37.95
103				138	1.369	28.068	84.123		36.30
	0							1.00	
105	N	LEU			0.165	27.313	82.368		37.66
106	CA	LEU			-0.617	28.512	82.249	1.00	
107	CB			139	-1.012	28.701	80.804		34.42
108	CG			139	0.147	29.153	79.918		35.08
109	CD1	LEU			-0.222	29.021	78.419	1.00	33.54
110	CD2	LEU			0.576	30.644	80.230	1.00	35.10
111	С			139	-1.861	28.421	83.112	1.00	36.45
112	0			139	-2.410	29.451	83.532	1.00	35.77
113	N	GLY			-2.322	27.205	83.377	1.00	36.33
114	CA	GLY			-3.533	27.031	84.172	1.00	36.31
115	С	GLY			-3.900	25.579	84.428	1.00	37.85
116	0	GLY			-3.285	24.651	83.886	1.00	
117	N	LYS	Α	141	-4.872	25.372	85.301	1.00	38.89
118	CA	LYS	Α	141	-5.255	24.016	85.681	1.00	40.43
119	CB	LYS			-5.479	23.905	87.204	1.00	41.81
120	CG	LYS	Α	141	-4.305	23.314	88.006	1.00	47.61
121	CD	LYS	Α	141	-4.581	23.141	89.534	1.00	54.52
122	CE	LYS	Α	141	-4.243	24.411	90.322	1.00	58.25
123	NZ	LYS	Α	141	-3.204	25.271	89.614	1.00	61.08
124	С	LYS	Α	141	-6.575	23.809	84.999	1.00	39.72
125	0	LYS	Α	141	-7.461	24.608	85.185	1.00	39.23
126	N	GLY	Α	142	-6.677	22.773	84.167		39.64
127	CA	GLY	Α	142	-7.934	22.410	83.523	1.00	40.24
128	С	GLY			-8.491	21.213	84.310	1.00	41.17
129	0	GLY	Α	142	-7.897	20.741	85.294	1.00	41.10
130	N	LYS	Α	143	-9.640	20.722	83.907	1.00	41.52
131	CA	LYS	Α	143	-10.245	19.612	84.630	1.00	42.27
132	СВ	LYS	Α	143	-11.686	19.435	84.202	1.00	43.00
133	CG	LYS	Α	143	-12.432	18.544	85.170	1.00	48.58
134	CD	LYS	Α	143	-13.719	18.034	84.570	1.00	52.87
135	CE	LYS	Α	143	-14.622	17.577	85.684	1.00	56.82
136	NΖ	LYS	Α	143	-14.896	16.117	85.592	1.00	61.41
137	С	LYS	Α	143	-9.471	18.292	84.453	1.00	41.56
138	0	LYS	Α	143	-9.248	17.572	85.412	1.00	40.75
139	N			144	-9.014	18.045	83.228		40.56
140	CA		Α	144	-8.344	16.807	82.827		40.12
141	СВ			144	-9.010	16.315	81.546		40.15
142	CG			144	-10.461	16.037	81.725		42.78
143	CD1	PHE	Α	144	-10.877	14.867	82.383	1.00	45.37

## FIGURE 3C

A	В	С	D	E	F	G	Н	I	J
144	CE1	PHE	Δ	144	-12.211	14.607	82.568	1 00	42.37
145	CZ	PHE			-13.160	15.517	82.120		44.22
146	CE2			144	-12.757	16.679	81.499		43.36
147	CD2	PHE			-11.420	16.948	81.315		39.89
148	CD2	PHE			-6.842	16.866	82.611		38.97
							82.150		
149	0			144	-6.253	15.909			36.84
150	N	GLY			-6.208	17.962	83.020		37.37
151	CA	GLY			-4.783	18.120	82.806		38.17
152	С	GLY			-4.486	19.606	82.814		37.75
153	0	GLY			-5.404	20.395	82.853		38.54
154	N	ASN			-3.230	19.999	82.753		38.01
155	CA	ASN			-2.930	21.412	82.804		37.94
156	СВ	ASN			-1.619	21.626	83.563		38.27
157	CG	ASN			-1.718	21.186	85.022		43.37
158	OD1	ASN			-2.704	21.454	85.695		49.18
159	ND2	ASN			-0.698	20.506	85.499		48.99
160	С	ASN	Α	146	-2.821	21.982	81.391		36.46
161	0	ASN	Α	146	-2.732	21.209	80.411	1.00	35.01
162	N	VAL			-2.830	23.317	81.293		34.34
163	CA	VAL	Α	147	-2.512	23.965	80.024		32.03
164	СВ	VAL	Α	147	-3.518	25.083	79.686	1.00	32.73
165	CG1	VAL	Α	147	-3.098	25.767	78.335	1.00	31.49
166	CG2	VAL	Α	147	-4.929	24.556	79.623	1.00	33.51
167	С	VAL	Α	147	-1.081	24.524	80.153	1.00	32.07
168	0	VAL	Α	147	-0.748	25.168	81.197	1.00	31.84
169	N	TYR	Α	148	-0.227	24.312	79.148	1.00	29.65
170	CA	TYR	Α	148	1.167	24.744	79.257	1.00	30.70
171	CB	TYR	Α	148	2.135	23.546	79.082	1.00	30.68
172	CG	TYR	Α	148	1.969	22.547	80.199	1.00	34.98
173	CD1	TYR	Α	148	1.006	21.542	80.117	1.00	36.63
174	CE1	TYR	Α	148	0.800	20.623	81.187	1.00	43.31
175	CZ	TYR	Α	148	1.568	20.721	82.344	1.00	43.61
176	ОН	TYR	Α	148	1.362	19.826	83.394	1.00	45.34
177	CE2	TYR	Α	148	2.513	21.730	82.456	1.00	43.40
178	CD2	TYR	Α	148	2.719	22.648	81.356	1.00	40.12
179	С	TYR	Α	148	1.532	25.740	78.197		30.72
180	0	TYR	Α	148	1.079	25.648	77.054		30.29
181	N	LEU	Α	149	2.386	26.675	78.554		30.08
182	CA	LEU			3.001	27.513	77.534		30.86
183	СВ	LEU			3.880	28.526	78.247		32.09
184	CG	LEU			4.108	29.924	77.676		36.09
185	CD1	LEU			5.567	30.516	77.808		34.85
186	CD2	LEU			3.332	30.344	76.361		32.07
187	C	LEU			3.902	26.615	76.717		29.91
188	0			149	4.557	25.743	77.269		31.11
189	N	ALA			4.008	26.837	75.417		29.95
190	CA	ALA			4.879	25.986	74.645		29.87
191	CB	ALA			4.091	24.697	74.127		29.08
192	С	ALA			5.435	26.770	73.456		30.54
193	0	ALA			4.860	27.774	72.966		29.82
194	N	ARG			6.558	26.299	72.900		30.55
エクセ	TA	DVID	$\overline{\Box}$	тОТ	0.550	20.299	12.330	1.00	50.55

#### FIGURE 3D

A	В	С	D	E	F	G	Н	I	J
195	CA	ARG	Α	151	7.164	26.847	71.809	1.00	32.81
196	СВ	ARG	Α	151	8.465	27.561	72.162	1.00	33.58
197	CG	ARG	Α	151	8.864	28.606	71.141	1.00	34.41
198	CD	ARG	Α	151	10.216	29.272	71.493	1.00	37.68
199	NE	ARG			11.314	28.358	71.774		41.98
200	CZ	ARG		151	12.579	28.754	71.840	1.00	
201	NH1	ARG	Α		12.855	30.033	71.642	1.00	
202	NH2	ARG	Α		13.554	27.891	72.109	1.00	
203	С	ARG			7.393	25.735	70.792	1.00	33.58
204	0	ARG			7.806	24.623	71.151		36.75
205	N	GLU	Α	152	6.998	26.037	69.557	1.00	
206	CA	GLU	Α	152	7.214	25.150	68.433	1.00	38.01
207	СВ	GLU	Α	152	6.339	25.554	67.232	1.00	38.19
208	CG	GLU	Α	152	6.245	24.450	66.177	1.00	44.01
209	CD	GLU	Α	152	7.475	24.363	65.241	1.00	48.90
210	OE1	GLU	Α	152	7.735	25.334	64.489	1.00	52.00
211	OE2	GLU	Α	152	8.192	23.320	65.250	1.00	51.05
212	С	GLU	Α	152	8.677	25.296	68.065	1.00	37.84
213	0	GLU	Α	152	9.161	26.382	67.791	1.00	38.28
214	N	LYS	Α	153	9.392	24.200	68.043	1.00	39.21
215	CA	LYS	Α	153	10.819	24.306	67.841	1.00	42.09
216	СВ	LYS	Α	153	11.481	22.967	68.153	1.00	42.63
217	CG	LYS	Α	153	11.928	22.851	69.590	1.00	48.61
218	CD	LYS	Α	153	11.539	21.510	70.175	1.00	55.42
219	CE	LYS	Α	153	11.720	20.374	69.179	1.00	60.62
220	NZ	LYS	Α	153	13.095	19.664	69.260	1.00	68.26
221	С	LYS	Α	153	11.287	24.885	66.509	1.00	42.57
222	0	LYS	Α	153	12.262	25.589	66.449	1.00	43.65
223	N	GLN	Α	154	10.603	24.623	65.421		43.01
224	CA	GLN			11.158	25.126	64.163		44.19
225	СВ	GLN			10.676	24.231	63.015		44.67
226	CG	GLN			11.442	22.952	63.045	1.00	
227	CD	GLN			11.408	22.213	61.740		60.70
228	OE1	GLN			10.328	21.982	61.174		66.15
229	NE2	GLN			12.586	21.838	61.246		64.53
230	С			154	10.856	26.600	63.884	1.00	
231	0	GLN			11.660	27.356	63.358		42.67
232	N			155	9.675	27.022	64.254		38.39
233	CA			155	9.313	28.371	63.946		35.68
234	CB			155	7.840	28.364	63.594		34.74
235	OG			155	7.196	27.875	64.746		34.70
236	С			155	9.532	29.313	65.140		33.68
237	0			155	9.505	30.517	64.946		33.85
238	N C7			156	9.672	28.739	66.331		32.82
239	CA			156	9.704	29.445	67.645		34.59
240 241	CB			156	10.858	30.467 29.876	67.753		34.66
241	CG			156	12.319		67.480 67.970		36.79 44.57
242	CD CE			156 156	13.429 14.696	30.907 31.115	67.056		44.57
243	CE NZ			156	14.787	32.563	66.539		46.31
244	N Z C			156	8.335	30.102	67.987		33.10
240		пто	А	100	0.333	30.102	01.901	1.00	22.10

## FIGURE 3E

A	В	С	D	E	F	G	Н	I	J
246	0	LYS	Α	156	8.218	31.065	68.804	1.00	31.56
247	N	PHE		157	7.302	29.553	67.386	1.00	
248	CA	PHE	Α	157	5.948	30.020	67.646	1.00	31.45
249	СВ	PHE	Α	157	5.016	29.469	66.575	1.00	
250	CG		Α	157	3.713	30.177	66.469	1.00	34.87
251	CD1	PHE	Α	157	3.527	31.155	65.492	1.00	38.48
252	CE1	PHE	Α	157	2.274	31.786	65.329	1.00	40.08
253	CZ	PHE	Α	157	1.209	31.427	66.143	1.00	37.15
254	CE2	PHE	Α	157	1.368	30.425	67.104	1.00	34.69
255	CD2	PHE	Α	157	2.644	29.795	67.253	1.00	36.13
256	С	PHE	Α	157	5.466	29.641	69.057	1.00	29.29
257	0	PHE	Α	157	5.395	28.469	69.412	1.00	29.48
258	N	ILE	Α	158	5.022	30.656	69.813	1.00	29.61
259	CA	ILE	Α	158	4.651	30.447	71.207	1.00	
260	СВ	ILE	Α	158	4.899	31.717	72.032	1.00	31.00
261	CG1	ILE	Α	158	6.366	31.797	72.339	1.00	36.27
262	CD1	ILE		158	6.687	30.925	73.512	1.00	
263	CG2	ILE			4.419	31.510	73.466	1.00	
264	С	ILE		158	3.209	30.163	71.230		29.07
265	0	ILE			2.473	30.911	70.644	1.00	
266	Ν	LEU		159	2.745	29.157	71.935	1.00	
267	CA	LEU		159	1.339	28.868	71.885	1.00	
268	СВ	LEU			1.085	27.936	70.692	1.00	
269	CG	LEU			1.953	26.777	70.259		34.00
270	CD1	LEU		159	1.782	25.602	71.203		35.94
271	CD2	LEU		159	1.737	26.341	68.787	1.00	
272	С			159	1.079	28.193	73.204		27.83
273	O			159	1.957	28.166	74.034		27.51
274 275	N C 7	ALA		160 160	-0.120	27.685 27.016	73.409 74.661	1.00	29.15
275	CA CB	ALA		160	-0.450 -1.651	27.684	75.323	1.00	
277	СВ	ALA			-0.818	25.602	74.297	1.00	
278	0	ALA			-1.472	25.371	73.269		31.99
279	N	LEU		161	-0.434	24.654	75.163		33.02
280	CA	LEU		161	-0.741	23.261	74.941		34.14
281	СВ	LEU		161	0.577	22.495	74.913	1.00	
282	CG	LEU		161	0.908	21.455	73.868	1.00	39.45
283		LEU			0.455	21.854	72.442		35.63
284		LEU			2.466	21.138	73.933		40.14
285	С			161	-1.648	22.780	76.036		33.03
286	0	LEU	Α	161	-1.271	22.762	77.217		33.04
287	N	LYS	Α	162	-2.885	22.456	75.657	1.00	31.43
288	CA	LYS	Α	162	-3.856	21.979	76.610	1.00	32.34
289	CB	LYS	Α	162	-5.251	22.451	76.196	1.00	32.99
290	CG	LYS	Α	162	-6.391	21.951	77.087		29.62
291	CD	LYS			-7.595	22.831	76.855		29.33
292	CE	LYS	А	162	-8.841	22.204	77.533		27.32
293	NZ			162	-10.098	22.987	77.412		31.96
294	С			162	-3.772	20.441	76.654		33.11
295	0			162	-4.017	19.775	75.666		33.31
296	Ν	VAL	А	163	-3.364	19.907	77.790	1.00	35.02

### FIGURE 3F

A	В	С	D	E	F	G	Н	I	J
207	C 7	7.77 T	7\	160	2 205	10 471	77 002	1 00	27 17
297	CA	VAL			-3.205	18.471	77.983		37.14
298	CB	LAV			-1.971	18.203	78.854	1.00	36.58
299	CG1	LAV			-1.720	16.660	79.039	1.00	37.74
300	CG2	VAL			-0.709	18.909	78.260	1.00	38.41
301	С	VAL			-4.445	17.854	78.653	1.00	37.59
302	0	VAL		163	-4.960	18.395	79.644	1.00	37.22
303	N	LEU			-4.977	16.767	78.073	1.00	39.14
304	CA			164	-6.104	16.048	78.686	1.00	39.01
305	СВ	LEU			-7.427	16.202	77.930	1.00	39.22
306	CG	LEU			-7.961	17.622	77.781	1.00	38.09
307	CD1	LEU			-7.363	18.125	76.508	1.00	38.01
308	CD2	LEU			-9.453	17.647	77.711	1.00	37.35
309	С			164	-5.759	14.562	78.783	1.00	
310	0	LEU			-5.369	13.952	77.798	1.00	38.76
311	N			165	-5.880	14.004	79.986	1.00	40.67
312	CA			165	-5.535	12.599	80.211	1.00	42.42
313	СВ			165	-5.191	12.355	81.686	1.00	42.83
314	CG	PHE		165	-3.815	12.784	82.030	1.00	46.45
315	CD1	PHE		165	-3.573	14.040	82.560	1.00	47.62
316	CE1			165	-2.290	14.434	82.868	1.00	47.96
317	CZ	PHE		165	-1.227	13.574	82.628	1.00	50.56
318	CE2	PHE		165	-1.446	12.349	82.067	1.00	48.72
319	CD2		Α	165	-2.740	11.951	81.775	1.00	48.08
320	С				-6.665	11.709	79.743	1.00	42.46
321	0		Α	165	-7.788	11.832	80.199	1.00	
322	N			166	-6.360	10.867	78.768	1.00	
323	CA			166	-7.342	9.957	78.209	1.00	45.50
324	СВ			166	-6.696	9.043	77.155	1.00	46.27
325	CG			166	-6.559	9.666	75.786	1.00	46.27
326	CD	LYS			-5.423	8.956	75.032	1.00	53.89
327	CE	LYS			-5.279	9.445	73.581	1.00	55.13
328	NZ			166	-5.709	8.444	72.569	1.00	59.86
329	С	LYS			-8.040	9.102	79.273	1.00	45.98
330	0	LYS			-9.230	8.981	79.250	1.00	46.56
331	N	ALA			-7.324	8.561	80.240	1.00	47.94
332	CA	ALA			-8.025	7.699	81.191	1.00	49.17
333	СВ	ALA			-7.091	7.201	82.220	1.00	49.16
334	С	ALA			-9.168	8.457			
335	0	ALA			-10.305	7.957	81.995		49.78
336	N			168	-8.859	9.696	82.218		49.84
337	CA			168	-9.787	10.502	82.960		49.29
338	СВ	GLN			-9.058	11.694	83.591		50.22
339	CG	GLN			-8.451	11.419	84.993		54.78
340	CD	GLN			-7.028	10.830	84.965		62.45
341	OE1	GLN			-6.053	11.569	84.788		65.02
342	NE2	GLN			-6.908	9.511	85.190		64.80
343	С	GLN			-10.953	10.939	82.088	1.00	
344	0			168	-12.085	10.976	82.553	1.00	
345	N			169	-10.702	11.245	80.814		48.22
346	CA			169	-11.808	11.676	79.964		48.39
347	СВ	LEU	Α	169	-11.322	12.112	78.575	1.00	47.89

### FIGURE 3G

A	В	С	D	E	F	G	Н	I	J
2.40	~~		-	1.60	10 644	10 461	70 220	1 00	40 67
348	CG	LEU			-10.644	13.461	78.330		49.67
349	CD1	LEU			-10.181	13.552	76.882	1.00	48.91
350	CD2	LEU			-11.615	14.580	78.615	1.00	
351	С	LEU		169	-12.819	10.538	79.785	1.00	
352	0	LEU		169	-14.027	10.733	79.875		47.83
353	N	ALA		170	-12.316	9.368	79.451	1.00	
354	CA	ALA		170	-13.220	8.238	79.195		48.55
355	СВ	ALA			-12.468	7.070	78.581	1.00	
356	С	ALA			-13.927	7.860	80.494		48.26
357	0	ALA			-15.118	7.692	80.501	1.00	
358	N	ALA			-13.207	7.806	81.606	1.00	48.63
359	CA	ALA			-13.857	7.578	82.885	1.00	
360	СВ	ALA			-12.858	7.685	84.058	1.00	
361	С	ALA			-14.996	8.561	83.082	1.00	
362	0	ALA			-16.113	8.179	83.429	1.00	48.35
363	N	ALA			-14.723	9.841	82.844	1.00	
364	CA	ALA			-15.740	10.846	83.012	1.00	
365	CB	ALA			-15.093	12.246	83.064	1.00	
366	С	ALA			-16.759	10.737	81.888	1.00	
367	0	ALA			-17.893	11.232	81.984	1.00	48.40
368	N	GLY			-16.371	10.067	80.815	1.00	48.12
369	CA	GLY			-17.262	9.907	79.674	1.00	
370 371	С	GLY GLY			-17.733 -18.926	11.166	78.995	1.00	47.73 49.07
372	0	VAL		173 174	-16.920 -16.790	11.308 12.075	78.705 78.736		46.88
373	N CA	VAL			-10.790 -17.030	13.322	78.021		45.99
374	CB	VAL			-16.674	14.572	78.873		45.74
375	CG1	VAL			-17.722	14.810	79.913	1.00	
376	CG2	VAL			-15.330	14.425	79.472	1.00	
377	C	VAL			-16.132	13.394	76.798	1.00	44.25
378	0	VAL			-15.792	14.483	76.300	1.00	
379	N	ALA			-15.708	12.236	76.322	1.00	
380	CA	ALA			-14.879	12.221	75.125	1.00	41.82
381	CB	ALA			-14.563	10.748	74.679	1.00	
382	C	ALA			-15.577	13.026	74.008	1.00	40.98
383	0	ALA			-14.920	13.683	73.189	1.00	
384	N	HIS			-16.899	13.030	74.009	1.00	
385	CA	HIS			-17.657		72.980		41.39
386	СВ	HIS			-19.146	13.385	73.068		41.58
387	CG	HIS			-19.803	13.903	74.318		45.86
388	ND1	HIS			-19.695	13.259	75.543		47.14
389	CE1	HIS			-20.355	13.949	76.460		47.79
390	NE2	HIS			-20.854	15.035	75.885		49.44
391	CD2	HIS			-20.532	15.023	74.545		46.34
392	C	HIS			-17.477	15.312	73.096		40.21
393	0	HIS			-17.529	16.043	72.107	1.00	38.56
394	N	GLN			-17.282	15.793	74.320	1.00	39.05
395	CA	GLN			-17.021	17.231	74.544		39.77
396	СВ	GLN			-17.008	17.567	76.019		38.88
397	CG	GLN			-18.343	17.312	76.675		38.17
398	CD	GLN	Α	177	-18.467	17.978	78.032		36.45

### FIGURE 3H

A	В	С	D	E	F	G	Н	I	J
399	OE1	GLN	Α	177	-19.540	18.436	78.382	1.00	43.55
400	NE2	GLN	Α	177	-17.393		78.801	1.00	32.42
401	С	GLN	Α	177	-15.672		73.966	1.00	39.55
402	0	GLN	Α	177	-15.519		73.379	1.00	40.58
403	N	LEU	Α	178	-14.691		74.144	1.00	38.53
404	CA	LEU	Α	178	-13.396		73.556	1.00	38.40
405	CB	LEU	Α	178	-12.332		73.974	1.00	37.56
406	CG	LEU	Α	178	-10.937	16.463	73.548	1.00	39.19
407	CD1	LEU	Α	178	-10.647		74.074	1.00	42.88
408	CD2	LEU	Α	178	-9.892		74.112	1.00	42.48
409	С	LEU	Α	178	-13.537		72.039	1.00	38.85
410	0	LEU	Α	178	-12.977	17.902	71.384	1.00	38.48
411	N	ARG		179	-14.362		71.478	1.00	38.80
412	CA	ARG		179	-14.528		70.027	1.00	38.95
413	СВ	ARG		179	-15.552		69.583	1.00	41.23
414	CG	ARG		179	-15.211		68.199	1.00	45.48
415	CD	ARG		179	-15.384		68.099	1.00	56.58
416	NE	ARG		179	-16.441		69.012	1.00	57.68
417	CZ	ARG		179	-16.275		69.973	1.00	57.26
418	NH1	ARG		179	-17.291		70.749	1.00	53.81
419	NH2	ARG		179	-15.093		70.159	1.00	59.58
420	С	ARG		179	-15.092		69.558	1.00	38.62
421	0	ARG		179	-14.762		68.508	1.00	38.21
422	N	ARG		180	-16.042		70.318	1.00	39.35
423	CA	ARG		180	-16.739		69.851	1.00	41.02
424	СВ	ARG		180	-18.096		70.575	1.00	41.10
425	CG	ARG		180	-19.359		69.686	1.00	48.65
426	CD	ARG		180	-20.364		70.125	1.00	56.75
427	NE	ARG		180	-20.662		71.551	1.00	60.82
428	CZ			180	-21.716		72.127	1.00	64.30
429	NH1	ARG		180	-21.941		73.430	1.00	64.17
430	NH2	ARG		180	-22.566		71.400	1.00	65.87
431 432	C O	ARG		180	-15.888 -15.924		69.923	1.00	39.65
432	N	ARG GLU		180 181			69.026	1.00	38.25
433	CA	GLU		181	-15.136 -14.302		71.003 71.254	1.00	39.01 38.98
435	CB	GLU			-13.453		72.514	1.00	39.58
					-13.433	22.429			
436 437	CG CD	GLU GLU			-11.926		72.937 74.396		41.25 44.88
438	OE1	GLU			-10.944		74.792		48.21
439	OE2	GLU		181	-12.528		75.192		45.90
440	C	GLU		181	-13.361		70.074	1.00	38.90
441	0	GLU			-13.111		69.576	1.00	
442	N			182	-12.803		69.651	1.00	
443	CA			182	-11.850		68.537	1.00	
444	CB			182	-11.090		68.390	1.00	
445	CG1			182	-10.416		66.980	1.00	
446	CG2			182	-10.051		69.506	1.00	38.26
447	C			182	-12.541		67.237	1.00	38.65
448	0			182	-12.119		66.516	1.00	39.07
449	N			183	-13.656		66.957		39.36

## FIGURE 3I

А	В	С	D	E	F	G	Н	I	J
450	CA	ALA	Ά	183	-14.312	20.503	65.679	1.00	40.14
451	СВ	ALA			-15.334	19.370	65.405		41.08
452	C	ALA			-14.965	21.870	65.636	1.00	40.80
453	0	ALA			-14.972	22.545	64.609	1.00	41.84
454	N			184	-15.524	22.312	66.748	1.00	38.99
455	CA			184	-16.157	23.595	66.678	1.00	39.48
456	CB			184	-17.210	23.754	67.766	1.00	38.90
457	CG1			184	-18.387	22.819	67.472	1.00	42.19
458	CD1	ILE			-19.459	22.799	68.584	1.00	
459	CG2	ILE			-17.715	25.164	67.777		40.73
460	C			184	-15.124	24.703	66.747		39.32
461	0			184	-15.148	25.635	65.929		38.88
462	N	GLN			-14.209	24.612	67.723	1.00	38.82
463	CA	GLN			-13.281	25.717	67.911	1.00	
464	CB	GLN			-12.446	25.531	69.185	1.00	
465	CG	GLN			-12.446	26.806	70.015	1.00	36.79
466	CD	GLN			-12.420	26.663	70.013	1.00	38.97
467	OE1	GLN			-11.023	27.519	71.599	1.00	35.32
468	NE2	GLN			-10.817	25.627	71.997	1.00	32.38
469	C	GLN			-12.337	25.905	66.754	1.00	38.81
470	0	GLN			-12.337	27.027	66.479	1.00	37.38
471	N			186	-11.936	24.823	66.083	1.00	39.57
472	CA			186	-11.940 $-10.957$	25.005	65.007	1.00	41.86
473	CB			186	-10.337	23.684	64.569	1.00	41.93
474	OG			186	-10.302	22.671	64.412	1.00	42.48
475	C			186	-11.509	25.748	63.798	1.00	
476	0			186	-10.761	26.297	63.798		43.08
477	N	HIS			-10.701	25.781	63.656		43.53
478	CA	HIS			-13.397	26.411	62.471		45.61
479	CB	HIS			-14.585	25.580	61.955	1.00	
480	CG	HIS			-14.173	24.264	61.396	1.00	52.65
481	ND1	HIS			-14.352	23.934	60.072	1.00	58.39
482	CE1			187	-13.863	22.725	59.855	1.00	
483	NE2			187	-13.354	22.269	60.986		59.03
484	CD2	HIS			-13.527	23.215	61.965	1.00	56.31
485	C	HIS			-13.815	27.843	62.684	1.00	44.76
486	0	HIS			-13.962	28.608	61.725		44.78
487	N	LEU			-13.984		63.945		44.38
488	CA			188	-14.351	29.612	64.257		43.43
489	CB			188	-14.767	29.748	65.747		43.01
490	CG			188	-15.964	28.891	66.146		43.56
491	CD1			188	-16.328	29.051	67.640		41.71
492	CD2	LEU			-17.109	29.282	65.302		41.54
493	C			188	-13.143	30.477	64.001		42.37
494	0			188	-12.036	30.079	64.321		43.11
495	N	ARG			-13.365	31.677	63.478		42.12
496	CA	ARG			-12.293	32.644	63.200		42.01
497	CB	ARG			-11.962	32.682	61.695		42.31
498	CG	ARG			-11.239	31.477	61.229	1.00	
499	CD			189	-9.871	31.267	61.898		46.81
500	NE			189	-9.128	30.280	61.109		54.20
5 5 5		\			3.120		505		

## FIGURE 3J

A	В	С	D	E	F	G	Н	I	J
501	CZ	ARG	Δ	189	-9.33	5 28.979	61.187	1 00	56.68
502	NH1	ARG			-8 <b>.</b> 64			1.00	
503	NH2	ARG			-10.23			1.00	57.84
504	C	ARG			-12.80			1.00	41.15
505	0	ARG			-13.55			1.00	
506	N	HIS			-13.33			1.00	
507		HIS			-12.40				38.65
508	CA CB	HIS		190					
509	СБ СG			190	-14.31			1.00	38.81
510		HIS			-14.92 -15.86				39.63
511	ND1			190					40.19
	CE1	HIS			-16.18			1.00	37.93
512	NE2	HIS			-15.48			1.00	36.58
513	CD2	HIS			-14.67			1.00	33.70
514	С	HIS			-11.90			1.00	37.98
515	0	HIS			-11.32			1.00	38.30
516	N	PRO		191	-11.64			1.00	38.45
517	CA	PRO		191	-10.58			1.00	36.82
518	CB	PRO			-10.61			1.00	37.97
519	CG	PRO			-12.03			1.00	38.87
520	CD	PRO			-12.25			1.00	38.97
521	С	PRO			-10.90			1.00	35.66
522	0	PRO			-9 <b>.</b> 99			1.00	34.96
523	N	ASN			-12.15			1.00	34.30
524	CA	ASN			-12.52			1.00	33.52
525	CB	ASN		192	-13.61				32.97
526 527	CG OD1	ASN		192 192	-13.20			1.00	35.71 35.61
528	ND2	ASN ASN			-12.28 -13.82			1.00	31.27
529	C	ASN			-13.82			1.00	32.20
530	0				-13.60			1.00	31.19
531	N	ASN		193	-13.80			1.00	30.72
532	CA			193	-12.50 -12.53			1.00	31.30
533	CB			193	-13.42			1.00	31.25
534	CG1	ILE			-14.86			1.00	32.94
535	CD1	ILE		193	-15.77			1.00	36.50
536	CG2	ILE		193	-13.37			1.00	29.33
537	C			193	-11.16			1.00	30.85
538	0			193	-10.47				31.20
539	N			194	-10.76				29.48
540	CA	LEU			-9.49				30.26
541	CB			194	-9 <b>.</b> 16				28.89
542	CG	LEU			-7 <b>.</b> 68				31.38
543	CD1	LEU			-6 <b>.</b> 95				27.79
544	CD2	LEU			-7 <b>.</b> 56				30.09
545	C	LEU			-9.41				30.59
546	0	LEU			-10.22				31.64
547	N	ARG			-8.41				31.20
548	CA	ARG			-8.12				32.25
549	СВ	ARG			-7 <b>.</b> 02				33.95
550	CG	ARG			-6.74				42.54
551	CD	ARG			-7.80				46.96

## FIGURE 3K

A	В	С	D	E	F		G		Н	I	J
552	NE	ARG	Δ	195	-7.275	5	29.900	6	3.663	1 00	52.66
553	CZ	ARG			-6.358		30.480		52.912	1.00	
554	NH1	ARG			-5.941		31.694		53.224	1.00	56.04
555	NH2	ARG			-5.861		29.867		51.844	1.00	60.45
556	C	ARG			-7.580		28.611		8.529	1.00	30.98
557	0	ARG			-6.771		28.614		59.450	1.00	28.95
558		LEU			-8.015		27.509				
559	N	LEU		196			26.226		57.984	1.00	31.25
560	CA CB			196	-7.440				58.277	1.00	31.50
		LEU		196	-8.517		25.265 23.870		58.720		32.30
561	CG CD1	LEU		196	-8.057				59.131	1.00	33.64
562		LEU			-9.058		23.370		0.151	1.00	36.24
563	CD2	LEU			-8.117		23.052		57.904	1.00	34.95
564	С	LEU			-6.795		25.867		6.932	1.00	35.11
565	0	LEU			-7.445		25.957		55.875	1.00	34.69
566	N	TYR			-5.509		25.518		56.972	1.00	
567	CA	TYR			-4.765		25.276		55.763		37.91
568	CB	TYR			-3.331		25.747		55.950	1.00	39.49
569	CG	TYR			-3.243		27.233		56.128	1.00	
570	CD1	TYR			-2.704		27.782		57.278	1.00	43.33
571	CE1	TYR			-2.619		29.122		57.439	1.00	
572	CZ	TYR			-3.072		29.953		6.451	1.00	44.37
573	OH	TYR			-2.949		31.310		56.604	1.00	48.37
574 575	CE2 CD2	TYR			-3.603		29.455		55.296 55.139	1.00	
576	CD2	TYR TYR			-3.697		28.087 23.826		55.380	1.00	
577	0	TYR		197	-4.762					1.00	38.77
578	N	GLY		198	-4.536 $-4.976$		23.490 22.955		54.216 56.351	1.00	39.64 37.60
579	CA	GLY			-5.013		21.553		6.019	1.00	38.52
580	CA	GLY			-4.785		20.771		57.265	1.00	38.86
581	0	GLY			-4.900		21.311		8.409	1.00	36.64
582	N	TYR			-4.428		19.511		57.066	1.00	38.68
583	CA	TYR			-4.334		18.597		8.185	1.00	
584	CB	TYR			-5.731		18.163		8.637	1.00	39.96
585	CG	TYR			-6.334		17.067		57.753		44.40
586	CD1	TYR			-7.074		17.385		6.618	1.00	
587	CE1	TYR		199	-7.626		16.382		55.807	1.00	
588	CZ	TYR		199	-7.420		15.058		6.132	1.00	50.76
589	OH	TYR			-7.947		14.040		55.357		58.47
590	CE2	TYR			-6.697		14.722		57.244		51.67
591	CD2	TYR			-6.160		15.736		8.060		46.05
592	C	TYR			-3.517		17.369		57.877		40.55
593	0	TYR			-3.291		17.055		6.728		40.45
594	N	PHE			-3.066		16.670		8.911		40.86
595	CA	PHE			-2.416		15.411		8.656		42.07
596	СВ	PHE			-0.963		15.636		8.198		41.03
597	CG	PHE			-0.122		16.422		59.173		44.63
598	CD1	PHE			0.713		15.760		0.035		42.87
599	CE1	PHE			1.515		16.436		0.934		44.73
600	CZ	PHE			1.477		17.801		1.010		43.50
601	CE2				0.655		18.492		0.162		43.78
602		PHE			-0.191		17.817		9.254		43.04

### FIGURE 3L

A	В	С	D	E	F	G	Н	I	J
603	С	חחב	7\	200	-2.610	14.522	69.888	1 00	42.82
604					-3.188				
	0			200		14.961	70.897	1.00	39.88
605	N	HIS		201	-2.268	13.251	69.770 70.911	1.00	44.66
606 607	CA				-2.394	12.350		1.00	48.80
	CB	HIS HIS		201	-3.807	11.739	70.991	1.00	49.16
608 609	CG ND1	HIS			-4.132 -3.940	10.793 9.429	69.870 69.956	1.00	53.25 57.68
610		HIS			-4.339	8.855	68.832	1.00	58.86
611	CE1 NE2	HIS			-4.339 -4.794	9.797	68.024	1.00	58.83
612	CD2	HIS			-4.676	11.018	68.650	1.00	57.09
613	CD2	HIS			-1.323	11.281	70.980	1.00	49.89
614	0	HIS			-0.807	10.810	69.960	1.00	50.59
615	N	ASP			-0.983	10.943	72.219	1.00	52.70
616	CA			202	-0.084	9.828	72.492	1.00	53.99
617	CB	ASP			1.241	10.287	73.079	1.00	54.12
618	CG	ASP			1.098	10.887	74.444	1.00	55.69
619	OD1	ASP			0.064	10.619	75.099	1.00	54.93
620	OD2	ASP			2.000	11.609	74.943	1.00	54.23
621	C	ASP			-0.819	8.790	73.330	1.00	54.16
622	0	ASP			-2.064	8.730	73.308	1.00	54.26
623	N	ALA			-0.084	7.976	74.067	1.00	54.51
624	CA	ALA			-0.738	6.843	74.732	1.00	54.56
625	СВ	ALA			0.314	5.869	75.285	1.00	54.78
626	C	ALA			-1.716	7.242	75.824	1.00	54.14
627	0	ALA			-2.869	6.753	75.887	1.00	54.14
628	N			204	-1.254	8.141	76.681	1.00	52.74
629	CA	THR	Α	204	-2.040	8.535	77.833	1.00	51.77
630	СВ	THR	Α	204	-1.114	8.467	79.073	1.00	52.77
631	OG1	THR	Α	204	-1.821	8.827	80.286	1.00	56.55
632	CG2	THR	Α	204	-0.003	9.483	78.940	1.00	51.61
633	С	THR	Α	204	-2.689	9.929	77.704	1.00	50.02
634	0			204	-3.546	10.290	78.496	1.00	48.39
635	N	ARG			-2.312	10.702	76.693	1.00	48.75
636	CA	ARG			-2.797	12.093	76.643	1.00	47.39
637	СВ	ARG			-1.740	13.047	77.192	1.00	47.22
638	CG	ARG			-1.295	12.746	78.573	1.00	50.14
639	CD	ARG			0.224	12.732	78.698	1.00	59.09
640	NE	ARG			0.805	13.946	79.262		65.81
641	CZ	ARG			2.118	14.116	79.455		71.17
642	NH1	ARG			2.587	15.256	79.974		73.74
643	NH2	ARG			2.968	13.142	79.123		72.85
644	С	ARG			-3.228	12.598	75.293	1.00	
645	0	ARG			-2.831	12.070	74.258		44.49
646	N	VAL			-4.119	13.582	75.354		42.03
647	CA			206	-4.578	14.339	74.206		40.02
648	CB			206	-6.136	14.273	74.061	1.00	
649	CG1	VAL			-6.638	15.182	72.954	1.00	
650 651	CG2			206	-6.580 -4.039	12.851	73.737	1.00	
651	С			206	-4.039	15.785	74.414		38.80
652 653	O N			<ul><li>206</li><li>207</li></ul>	-3.996 -3.593	16.298 16.409	75.539 73.341		38.31 37.44
654	CA			207	-3.593 -2.976	17.737	73.430		38.03
004	CA	TIL	$\Box$	201	2.3/0	11.131	10.400	<b>1.</b> 00	50.05

#### FIGURE 3M

А	В	С	D	E		F	G	Н		I	J
655	СВ	TYR	Α	207	-1	1.549	17.670	72.9	968	1.00	36.40
656	CG	TYR	Α	207		0.688	16.778	73.	766	1.00	39.00
657	CD1	TYR	Α	207	-(	0.010	17.249	74.8	381	1.00	39.70
658	CE1	TYR	Α	207	(	0.818	16.417	75.5	590	1.00	44.38
659	CZ	TYR	Α	207	(	0.948	15.092	75.2	187	1.00	45.91
660	ОН	TYR	Α	207	-	1.734	14.246	75.9	900	1.00	50.45
661	CE2	TYR	Α	207	(	.290	14.609	74.0	90	1.00	43.62
662	CD2	TYR	Α	207	-(	.539	15.439	73.3	398	1.00	40.40
663	С	TYR	Α	207	-(	3.595	18.728	72.5	511	1.00	37.21
664	0	TYR	Α	207	-(	3.384	18.643	71.2	286	1.00	39.25
665	N	LEU	Α	208		1.323	19.685	73.0	)49	1.00	35.21
666	CA	LEU	Α	208	- 4	1.858	20.693	72.1	172	1.00	32.76
667	СВ	LEU	Α	208	- (	5.177	21.235	72.	710	1.00	32.84
668	CG	LEU	Α	208		7.403	20.429	72.3	312	1.00	36.54
669	CD1	LEU	Α	208		7.148	18.880	72.2	249	1.00	39.94
670	CD2	LEU	Α	208	- {	3.584	20.792	73.2	169	1.00	34.97
671	С	LEU	Α	208	-(	3.851	21.827	71.9	975	1.00	31.94
672	0	LEU	Α	208	-(	3.292	22.378	72.9	960	1.00	31.89
673	N	ILE	Α	209	-(	3.605	22.175	70.	710	1.00	27.64
674	CA	ILE	Α	209	-2	2.719	23.286	70.3	374	1.00	29.03
675	СВ	ILE	Α	209	-2	2.034	23.047	69.0	043	1.00	29.46
676	CG1	ILE	Α	209	- 2	1.424	21.632	68.9	983	1.00	33.03
677	CD1	ILE	Α	209	-(	0.629	21.353	67.6	516	1.00	36.54
678	CG2	ILE	Α	209	-(	.996	24.092	68.8	333	1.00	27.57
679	С	ILE	Α	209	-(	3.518	24.572	70.2	249	1.00	29.27
680	0	ILE	Α	209	- 4	1.206	24.763	69.2	258	1.00	30.08
681	N	LEU	Α	210	-(	3.372	25.462	71.2	226	1.00	27.89
682	CA	LEU	Α	210	- 2	4.143	26.671	71.3	304	1.00	28.36
683	СВ	LEU	Α	210	- 2	1.768	26.757	72.	729	1.00	26.97
684	CG	LEU	Α	210	- į	5.603	25.569	73.2	209	1.00	31.79
685	CD1	LEU	Α	210	- (	5.165	25.926	74.6	513	1.00	31.27
686	CD2	LEU	Α	210	- (	5.798	25.282	72.2	204	1.00	34.08
687	С	LEU	Α	210	-(	3.346	27.967	71.0	066	1.00	26.61
688	0	LEU	Α	210	-2	2.177	28.060	71.3	382	1.00	27.93
689	N	GLU	Α	211	-(	3.994	28.972	70.5	520	1.00	29.15
690	CA	GLU	Α	211	-(	3.501	30.350	70.6	521	1.00	29.81
691	СВ	GLU	Α	211		1.498	31.350	70.0	)47	1.00	31.22
692	CG	GLU	Α	211	-(	3.984	32.779	70.0	020	1.00	35.70
693	CD	GLU	Α	211	- <u>:</u>	5.147	33.799	70.0	050	1.00	39.08
694	OE1	GLU	Α	211	- 4	1.932	34.950	70.4	189	1.00	43.39
695	OE2	GLU	Α	211	- 6	5.288	33.455	69.6	553	1.00	38.36
696	С	GLU	Α	211	-(	3.161	30.663	72.1	128	1.00	29.58
697	0	GLU	Α	211	-(	3.948	30.404	73.0	14	1.00	28.54
698	N	TYR	Α	212	-1	1.957	31.153	72.3	381	1.00	28.23
699	CA	TYR	Α	212		1.550	31.606	73.7	725	1.00	28.20
700	СВ			212	-(	0.028	31.697	73.7	739	1.00	28.08
701	CG			212		592	32.494	74.8	374		29.44
702	CD1			212		1.521	33.489	74.6			30.49
703	CE1			212		2.131	34.197	75.6			36.30
704	CZ			212	-	1.773	33.945	76.9	903	1.00	33.49
705	ОН	TYR	Α	212	2	2.383	34.655	77.8	387	1.00	37.20

## FIGURE 3N

A	В	С	D	E	F	G	Н	I	J
706	CE2	TYR	Α	212	0.802	32.977	77.225	1.00	33.16
707	CD2	TYR			0.234	32.258	76.188		28.40
708	C			212	-2.183	33.022	74.034	1.00	
709	0	TYR			-2.089	33.924	73.211	1.00	27.53
710	N	ALA			-2.836	33.156	75.205	1.00	
711	CA	ALA			-3.431	34.424	75.650	1.00	30.33
712	CB	ALA			-4.884	34.284	76.103	1.00	
713	C	ALA			-2.550	34.953	76.780	1.00	30.02
714	0	ALA			-2.634	34.540	77.872	1.00	31.02
715	N			214	-1.720	35.904	76.442	1.00	31.54
716	CA	PRO			-0.632	36.365	77.313	1.00	32.57
717	CB	PRO			0.219	37.264	76.395	1.00	32.48
718	CG	PRO			-0.495	37.305	75.047	1.00	35.80
719	CD	PRO			-1.853	36.639	75.171	1.00	30.79
720	C	PRO			-1.070	37.096	78.596		34.06
721	0	PRO			-0.408	36.972	79.644		35.53
722	N	LEU			-2.187	37.789	78.548	1.00	33.98
723	CA	LEU			-2.167	38.503	79.718	1.00	36.04
724	CB	LEU			-3.341	39.786	79.716	1.00	34.70
725	CG	LEU			-2.394	41.003	79.195	1.00	36.83
726	CD1	LEU				40.725	78.377	1.00	35.83
727	CD1	LEU			-1.157 -3.180		78.627	1.00	35.88
728	CD2	LEU				42.190		1.00	
729	0			215	-3.521 -4.121	37.689 38.247	80.677 81.571		35.81 35.82
730				216		36.381			
731	N CA	GLY			-3.603	35.503	80.470	1.00	35.32
732	CA	GLY			-4.326 -5.848	35.530	81.372 81.287	1.00	34.32 32.64
733	0			216	-6.426	35.895	80.257	1.00	32.48
734	N			217	-6.500	35.138	82.367	1.00	31.56
735	CA	THR			-7 <b>.</b> 962	35.119	82.396	1.00	31.29
736	CB			217	-8.511	33.951	83.212	1.00	32.13
737	OG1	THR			-8.082	34.088	84.587	1.00	30.67
738	CG2	THR			-7.974	32.629	82.730	1.00	31.12
739	C	THR			-8.613	36.355	83.020	1.00	31.68
740	0	THR			-8.041	37.069	83.856	1.00	28.84
741	N	VAL			-9.881	36.498	82.686	1.00	30.86
742	CA	VAL			-10.694	37.528	83.283	1.00	32.14
743	CB	VAL			-11.953		82.526		33.13
744		VAL			-12.978	38.466	83.328		35.75
745		VAL			-11.616	38.289	81.172		31.98
746	CGZ			218	-10.920	37.150	84.768		32.06
747	0			218	-11.039	38.023	85.642		32.00
748	N			219	-10.958	35.849	85.032		32.11
749	CA			219	-11.062	35.374	86.402		33.66
750	CB			219	-11.049	33.838	86.406	1.00	33.98
751	СБ			219	-11.116	33.234	87.785	1.00	35.90
752	CD1			219	-12.335	32.895	88.354	1.00	38.53
753	CE1			219	-12.333	32.339	89.620		46.18
754	CZ			219	-12.412	32.339	90.335		47.58
755	OH			219	-11.326	31.532	91.592		53.35
756	CE2			219	-10.001	32.451	89.785		42.92
150	CBZ	TIK	Ч	Z 1 9	-10.001	JZ.4JI	09.700	1.00	44.94

## FIGURE 30

A	В	С	D	E	F	G	Н	I	J
757	CD2	TYR	Δ	219	-9.954	32.999	88.517	1.00	37.24
758	C			219	-9.883	35.936	87.269		33.62
759	0			219	-10.105	36.423	88.379	1.00	33.27
760	N	ARG			-8.703	35.924	86.725	1.00	34.37
761	CA	ARG			-7 <b>.</b> 506	36.322	87.508	1.00	36.06
762	CB	ARG			-6.243	35.827	86.810	1.00	37.28
763	СБ СG				-5.058	35.372	87.750	1.00	44.07
764	CD	ARG ARG			-3.665				53.39
765	NE	ARG				35.138 36.401	87.075 86.587		57.56
766		ARG			-3.131 -3.067	36.736	85.300	1.00	
767	CZ	ARG			-2.583	37.921		1.00	63.45
	NH1						84.937		62.86
768	NH2	ARG			-3.473	35.882	84.365		65.24
769	С	ARG			-7.561 -7.328	37.846	87.621	1.00	35.84
770	0	ARG				38.467	88.683	1.00	
771	N	GLU			-7.928	38.427	86.490	1.00	
772	CA	GLU			-8.145	39.852	86.355	1.00	38.35
773	CB	GLU			-8.573	40.154	84.930	1.00	39.07
774	CG	GLU			-8.452	41.597	84.521	1.00	47.19
775	CD OF1	GLU			-7.205	42.221	85.080	1.00	57.25
776 777	OE1	GLU			-6.259	42.459	84.291	1.00	60.27
	OE2	GLU			-7.178	42.474	86.314	1.00	62.91
778	С	GLU			-9.149	40.339	87.416	1.00	38.74
779	O	GLU		221	-8.832	41.307	88.117	1.00	38.67
780	N				-10.296	39.663	87.575	1.00	37.69
781 782	CA	LEU LEU			-11.188 -12.513	40.011 39.256	88.668 88.615	1.00	39.29 40.21
783	CB CG	LEU			-13.754	39.230	88.040	1.00	
784	CD1	LEU			-13.754	41.386	88.378	1.00	
785	CD1	LEU			-13.856	39.644	86.553	1.00	52.48
786	C	LEU			-10.654	39.766	90.079	1.00	40.79
787	0	LEU			-10.981	40.510	91.025	1.00	40.30
788	N	GLN			-9.904	38.712	90.272	1.00	40.08
789	CA	GLN			-9.456	38.509	91.612	1.00	43.39
790	CB	GLN			-9.120	37.025	91.889	1.00	44.71
791	CG	GLN			-7 <b>.</b> 754	36.535	91.538	1.00	49.87
792	CD	GLN			-7.627	34.996	91.712	1.00	56.56
793	OE1	GLN			-6.942	34.309	90.918	1.00	58.11
794		GLN			-8.286		92.747		58.77
795	С	GLN			-8.380	39.560	91.978		43.05
796	0			223	-8.307	39.976	93.113		43.64
797	N			224	-7.673	40.083	90.988	1.00	
798	CA			224	-6.690	41.126	91.203	1.00	
799	СВ	LYS			-5.815	41.282	89.985		43.53
800	CG	LYS			-4.818	42.422	90.066		48.88
801	CD	LYS			-4.028	42.585	88.762		53.83
802	CE	LYS			-4.857	43.218	87.650		57.23
803	NZ			224	-4.028	43.546	86.442		60.62
804	С			224	-7.356	42.461	91.560	1.00	
805	0			224	-7.042	43.032	92.599	1.00	
806	N	LEU	Α	225	-8.297	42.913	90.732	1.00	40.83
807	CA	LEU	Α	225	-9.019	44.181	90.897	1.00	41.08

### FIGURE 3P

А	В	С	D	E	F	G	Н	I	J
808	СВ	LEU	Α	225	-9.501	44.691	89.533	1.00	39.93
809	CG	LEU	Α	225	-8.469	45.241	88.540	1.00	43.97
810	CD1	LEU	Α	225	-9.133	45.930	87.345	1.00	46.75
811	CD2	LEU	Α	225	-7.332	46.154	89.189	1.00	43.17
812	С	LEU	Α	225	-10.254	44.157	91.818	1.00	40.68
813	0	LEU	Α	225	-10.784	45.218	92.182	1.00	40.10
814	N	SER	Α	226	-10.732	42.961	92.147	1.00	40.56
815	CA	SER	Α	226	-11.977	42.780	92.913	1.00	41.73
816	СВ	SER	Α	226	-11.943	43.579	94.225	1.00	43.22
817	OG	SER	Α	226	-12.999	43.112	95.048	1.00	50.73
818	С	SER	Α	226	-13.295	43.050	92.126	1.00	40.15
819	0	SER	Α	226	-14.238	42.256	92.215	1.00	40.02
820	N	LYS	Α	227	-13.373	44.163	91.397	1.00	38.66
821	CA	LYS	Α	227	-14.500	44.424	90.506	1.00	38.28
822	СВ	LYS	Α	227	-15.744	44.876	91.241	1.00	39.83
823	CG	LYS	Α	227	-15.527	46.112	92.107	1.00	43.19
824	CD	LYS	Α	227	-16.763	46.395	92.964	1.00	47.23
825	CE	LYS	Α	227	-17.009	47.898	93.037	1.00	50.59
826	NZ	LYS	Α	227	-15.847	48.527	93.755	1.00	50.07
827	С	LYS	Α	227	-14.057	45.437	89.453	1.00	37.32
828	0	LYS	Α	227	-13.032	46.114	89.637	1.00	35.43
829	N	PHE	Α	228	-14.784	45.541	88.339	1.00	34.98
830	CA	PHE	Α	228	-14.287	46.384	87.241	1.00	34.36
831	СВ	PHE	Α	228	-14.483	45.686	85.908	1.00	32.60
832	CG	PHE	Α	228	-13.706	44.403	85.761	1.00	32.22
833	CD1	PHE	Α	228	-12.556	44.214	86.480	1.00	30.96
834	CE1	PHE	Α	228	-11.797	43.063	86.350	1.00	34.49
835	CZ	PHE	Α	228	-12.178	42.076	85.495	1.00	33.23
836	CE2	PHE	Α	228	-13.374	42.246	84.752	1.00	34.03
837	CD2	PHE		228	-14.105	43.409	84.862	1.00	33.41
838	С	PHE		228	-15.057	47.675	87.146	1.00	35.43
839	0	PHE	Α	228	-16.228	47.733	87.549	1.00	34.99
840	N	ASP		229	-14.441	48.714	86.591	1.00	36.24
841	CA	ASP	Α	229	-15.233	49.943	86.453	1.00	38.49
842	СВ	ASP	Α	229	-14.302	51.205	86.331	1.00	39.70
843	CG			229	-13.484	51.241	85.072	1.00	44.65
844	OD1	ASP	Α	229	-13.729	50.465	84.121	1.00	47.75
845	OD2	ASP			-12.527	52.046	84.948		52.81
846	С			229	-16.211	49.721	85.300		37.35
847	0			229	-16.187	48.669	84.633	1.00	35.10
848	N			230	-17.038	50.715	85.027	1.00	37.87
849	CA			230	-18.077	50.513	84.040	1.00	37.66
850	СВ			230	-19.054	51.668	84.115	1.00	
851	CG			230	-19.840	51.650	85.412		42.58
852	CD			230	-21.045	52.566	85.320	1.00	
853	OE1			230	-22.168	52.129	85.629		52.06
854	OE2			230	-20.868	53.740	84.896	1.00	
855	С			230	-17.483	50.440	82.659	1.00	36.98
856	0			230	-18.015	49.782	81.767	1.00	34.19
857	N			231	-16.382	51.159	82.461		36.82
858	CA	GLN	Α	231	-15.764	51.174	81.152	1.00	36.74

# FIGURE 3Q

859         CB         GLN         A         231         -14.587         52.171         81.128         1.00         37.58           860         CG         GLN         A         231         -14.995         53.671         81.393         1.00         43.18           861         CD         GLN         A         231         -15.731         53.743         83.729         1.00         42.61           863         NE2         GLN         A         231         -15.731         53.743         83.729         1.00         47.58           864         C         GLN         A         231         -15.212         49.784         80.817         1.00         35.85           865         O         GLN         A         232         -14.495         49.186         81.746         1.00         33.54           867         CA         ARG         A         232         -12.832         47.928         81.426         1.00         33.54           868         CB         ARG         A         232         -12.832         47.530         82.347         1.00         36.13           870         CD         ARG         A         232         -14.931 <th>A</th> <th>В</th> <th>С</th> <th>D</th> <th>E</th> <th>F</th> <th>G</th> <th>Н</th> <th>I</th> <th>J</th>	A	В	С	D	E	F	G	Н	I	J
860         CG         GLN A 231         -14.995         53.671         81.393         1.00         43.18           861         CD         GLN A 231         -16.011         53.956         82.522         1.00         46.32           863         NE2         GLN A 231         -17.181         53.743         83.729         1.00         47.58           864         C         GLN A 231         -15.212         49.784         80.817         1.00         35.85           865         O         GLN A 231         -15.382         49.294         79.724         1.00         36.28           867         CA         ARG A 232         -12.3858         47.928         81.426         1.00         33.54           868         CB         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -12.260         46.109         83.323         1.00         49.70           871         NE         ARG A 232         -14.934         46.602         83.368         1.00         49.70           872         CZ         ARG A 232         -8.817         45.862         2.371         1.00         55.78 </td <td>0.50</td> <td>CD.</td> <td>OT N</td> <td>70</td> <td>0.01</td> <td>14 507</td> <td>FO 171</td> <td>01 100</td> <td>1 00</td> <td>27 55</td>	0.50	CD.	OT N	70	0.01	14 507	FO 171	01 100	1 00	27 55
861         CD         GLN         A         231         -16.011         53.954         82.522         1.00         46.32           862         OE1         GLN         A         231         -17.181         53.743         83.729         1.00         42.61           864         C         GLN         A         231         -15.212         49.784         80.817         1.00         35.85           865         O         GLN         A         231         -15.212         49.784         80.817         1.00         35.85           866         N         ARG         A         232         -14.495         49.186         81.746         1.00         33.62           868         CB         ARG         A         232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG         A         232         -11.433         45.610         83.520         1.00         40.91           871         NE         ARG         A         232         -14.433         45.610         83.520         1.00         49.70           872         CZ         ARG A         232         -14.433 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
862         OE1         GLN A 231         -15.731         53.743         83.729         1.00         42.61           863         NEZ         GLN A 231         -17.181         54.488         82.121         1.00         47.58           865         O         GLN A 231         -15.212         49.784         80.817         1.00         35.88           866         N         ARG A 232         -14.495         49.186         81.746         1.00         33.62           867         CA         ARG A 232         -13.858         47.928         81.426         1.00         33.54           869         CG         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -10.425         46.602         83.868         1.00         49.70           872         CZ         ARG A 232         -9.221         46.706         83.323         1.00         55.97           873         NH1 ARGA         232         -9.421         46.706         83.368         1.00         31.99           874         NH2         ARG         232         -14.931         46.853         81.2371         1.00										
863         NE2         GLN A 231         -17.181         54.488         82.121         1.00         47.58           864         C         GLN A 231         -15.312         49.784         80.817         1.00         35.85           866         N         ARG A 232         -15.382         49.294         79.724         1.00         33.62           867         CA         ARG A 232         -12.832         47.928         81.426         1.00         33.54           868         CB         ARG A 232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -10.425         46.602         83.520         1.00         49.70           871         NE         ARG A 232         -8.817         45.862         82.371         1.00         53.98           873         NH1         ARG A 232         -8.409         47.659         83.755         1.00         55.76           875         C         ARG A 232         -14.931         46.852         80.341         1.00         30.54 <td></td>										
864         C         GLN A 231         -15.212         49.784         80.817         1.00         35.85           865         O         GLN A 231         -15.382         49.294         79.724         1.00         36.28           866         N         ARG A 232         -14.495         49.186         81.746         1.00         33.55           868         CB         ARG A 232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -10.425         46.602         83.868         1.00         49.70           871         NE         ARG A 232         -9.221         46.706         83.323         1.00         52.36           873         NH1         ARG A 232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG A 232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG A 232         -14.931         46.853         81.238         1.00         31.99 <td></td>										
865         O         GLN A 231         -15.382         49.294         79.724         1.00         36.28           866         N         ARG A 232         -14.495         49.186         81.746         1.00         33.62           867         CA         ARG A 232         -13.858         47.928         81.426         1.00         33.54           869         CG         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -11.433         45.610         83.323         1.00         49.70           871         NE         ARG A 232         -10.425         46.602         83.868         1.00         49.70           872         CZ         ARG A 232         -9.221         46.706         83.323         1.00         53.98           873         NH1         ARG A 232         -8.409         47.659         83.757         1.00         55.77           875         C         ARG A 232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG A 233         -17.071         45.931         82.002         1.00         30.48										
866         N         ARG A 232         -14.495         49.186         81.746         1.00         33.62           867         CA         ARG A 232         -13.858         47.928         81.426         1.00         33.54           868         CB         ARG A 232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG A 232         -10.425         46.602         83.520         1.00         49.70           871         NE         ARG A 232         -9.221         46.706         83.323         1.00         52.36           873         NH1         ARG A 232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG A 232         -14.931         46.853         81.238         1.00         31.99           875         C         ARG A 232         -14.931         46.890         82.072         1.00         30.75           878         C         THR A 233         -17.071         45.953         84.337         1.00         30.48 <td></td>										
867         CA         ARG         A 232         -13.858         47.928         81.426         1.00         33.95           868         CB         ARG         A 232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG         A 232         -11.433         45.610         83.520         1.00         40.91           871         NE         ARG         A 232         -10.425         46.602         83.868         1.00         49.70           872         CZ         ARG         A 232         -9.221         46.706         83.323         1.00         53.98           874         NH2         ARG         A 232         -9.221         46.706         83.757         1.00         55.77           875         C         ARG         A 232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG         A 232         -14.813         46.053         81.238         1.00         30.75           878         CA         THR         A 233         -17.071         45.931         82.002         1.00         30.48           879         CB										
868         CB         ARG         A 232         -12.832         47.530         82.509         1.00         33.54           869         CG         ARG         A 232         -12.260         46.109         82.347         1.00         36.13           871         NE         ARG         A 232         -10.425         46.602         83.568         1.00         49.70           872         CZ         ARG         A 232         -9.221         46.706         83.323         1.00         52.36           873         NH1         ARG         A 232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG         A 232         -8.409         47.659         83.757         1.00         53.98           875         C         ARG         A 232         -14.931         46.853         81.238         1.00         31.18           877         N         THR         A 233         -15.971         46.890         82.072         1.00         30.75           878         CA         THR         A 233         -17.071         45.931         82.002         1.00         30.48           879         CB										
869         CG         ARG         A 232         -12.260         46.109         82.347         1.00         36.13           870         CD         ARG         A 232         -11.433         45.610         83.520         1.00         40.91           871         NE         ARG         A 232         -10.425         46.602         83.868         1.00         49.70           873         NH1         ARG         A 232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG         A 232         -8.409         47.659         83.757         1.00         55.77           875         C         ARG         A 232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG         A 232         -14.813         46.023         80.341         1.00         30.75           878         C         THR         A 233         -17.071         45.931         82.002         1.00         30.48           879         CB         THR         A 233         -17.761         45.931         82.986         1.00         28.26           82         THR										
870         CD         ARG         A         232         -11.433         45.610         83.520         1.00         40.91           871         NE         ARG         A         232         -9.221         46.602         83.868         1.00         49.70           873         NH1         ARG         A         232         -8.817         45.862         82.371         1.00         55.77           875         C         ARG         A         232         -8.409         47.659         83.757         1.00         55.77           876         O         ARG         A         232         -14.813         46.833         81.238         1.00         31.98           877         N         THR         A         233         -15.971         46.890         82.072         1.00         30.75           878         CA         THR         A         233         -17.071         45.931         82.002         1.00         30.48           879         CB         THR         A         233         -17.071         45.931         82.002         1.00         30.41           870         CB         THR         A         233         -17.071										
871         NE         ARG         A         232         -9.221         46.602         83.868         1.00         49.70           872         CZ         ARG         A         232         -9.221         46.706         83.323         1.00         52.38           873         NH1         ARG         A         232         -8.409         47.659         83.757         1.00         55.77           875         C         ARG         A         232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG         A         232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG         A         232         -14.813         46.023         80.341         1.00         31.18           877         N         THR         A         233         -17.071         45.931         82.002         1.00         30.75           878         CA         THR         A         233         -17.464         45.953         84.337         1.00         28.281           881         CG         THR         A         233         -17.7937										
872         CZ         ARG         A         232         -9.221         46.706         83.323         1.00         52.36           873         NH1         ARG         A         232         -8.817         45.862         82.371         1.00         53.98           874         NH2         ARG         A         232         -8.409         47.659         83.757         1.00         31.99           876         O         ARG         A         232         -14.813         46.023         80.341         1.00         31.18           877         N         THR         A         233         -17.071         45.931         82.002         1.00         30.75           878         CA         THR         A         233         -17.071         45.931         82.002         1.00         30.75           878         CA         THR         A         233         -17.071         45.931         82.002         1.00         30.75           879         CB         THR         A         233         -17.783         46.522         80.670         1.00         29.48           881         CG2         THR A         233         -17.783 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
873         NH1         ARG         A         232         -8         409         47.659         83.757         1.00         55.77           875         C         ARG         A         232         -8         409         47.659         83.757         1.00         55.77           876         O         ARG         A         232         -14.931         46.853         81.238         1.00         31.99           877         N         THR         A         233         -15.971         46.890         82.072         1.00         30.75           878         CA         THR         A         233         -18.080         46.242         83.085         1.00         31.41           880         OG1         THR         A         233         -17.464         45.953         84.337         1.00         28.26           881         CG2         THR         A         233         -17.783         46.052         80.670         1.00         30.81           881         CG2         THR         A         233         -17.783         46.052         80.670         1.00         30.81           883         C         ALA         A <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
874         NH2         ARG         A         232         -8.409         47.659         83.757         1.00         55.77           875         C         ARG         A         232         -14.931         46.853         81.238         1.00         31.18           876         O         ARG         A         232         -14.813         46.023         80.341         1.00         31.18           877         N         THR         A         233         -15.971         46.890         82.072         1.00         30.78           878         CA         THR         A         233         -17.071         45.931         82.002         1.00         30.48           880         OGI         THR         A         233         -17.464         45.953         84.337         1.00         28.31           881         CG         THR         A         233         -17.783         45.050         79.937         1.00         29.48           884         N         ALA         A         234         -18.959         47.533         79.118         1.00         30.91           885         CA         ALA         A         234         -18.959										
875         C         ARG         A         232         -14.931         46.853         81.238         1.00         31.99           876         O         ARG         A         232         -14.813         46.023         80.341         1.00         31.18           877         N         THR         A         233         -17.071         45.931         82.002         1.00         30.48           879         CB         THR         A         233         -17.464         45.953         84.337         1.00         28.31           881         CG2         THR         A         233         -17.464         45.953         84.337         1.00         28.31           881         CG2         THR         A         233         -17.783         46.052         80.670         1.00         30.81           882         C         THR         A         233         -17.783         46.052         80.670         1.00         30.18           883         O         THR         A         233         -17.783         46.052         80.670         1.00         30.12           885         CA         ALA         A         234         -18.959										
876         O         ARG         A         232         -14.813         46.023         80.341         1.00         31.18           877         N         THR         A         233         -15.971         46.890         82.072         1.00         30.75           878         CA         THR         A         233         -17.071         45.931         82.002         1.00         30.48           879         CB         THR         A         233         -17.464         45.953         84.337         1.00         28.26           880         OG1         THR         A         233         -17.783         46.052         80.670         1.00         28.26           882         C         THR         A         233         -17.937         45.050         79.937         1.00         29.48           884         N         ALA         A         234         -18.283         47.261         80.402         1.00         30.12           885         CA         ALA         A         234         -18.959         47.533         79.18         1.00         30.12           886         CB         ALA         A         234         -18.914										
877         N         THR A 233         -15.971         46.890         82.072         1.00 30.75           878         CA         THR A 233         -17.071         45.931         82.002         1.00 30.48           879         CB         THR A 233         -18.080         46.242         83.085         1.00 31.41           880         OG1         THR A 233         -17.464         45.953         84.337         1.00 28.31           881         CG2         THR A 233         -17.783         46.052         80.670         1.00 30.81           883         O         THR A 233         -17.783         46.052         80.670         1.00 30.12           884         N         ALA A 234         -18.283         47.261         80.402         1.00 30.12           885         CA         ALA A 234         -18.959         47.533         79.118         1.00 30.91           886         CB         ALA A 234         -18.104         47.102         77.946         1.00 30.58           887         C         ALA A 234         -18.104         47.102         77.946         1.00 30.58           888         O         ALA A 235         -16.815         47.389         78.028         1.00										
878         CA         THR A 233         -17.071         45.931         82.002         1.00 30.48           879         CB         THR A 233         -18.080         46.242         83.085         1.00 31.41           880         OGI THR A 233         -17.464         45.953         84.337         1.00 28.31           881         CG2 THR A 233         -17.783         46.052         80.670         1.00 30.81           883         O THR A 233         -17.937         45.050         79.937         1.00 29.48           884         N ALA A 234         -18.283         47.261         80.402         1.00 30.12           885         CA ALA A 234         -18.959         47.533         79.118         1.00 30.91           886         CB ALA A 234         -18.959         47.533         79.118         1.00 30.91           887         C ALA A 234         -18.611         46.555         76.947         1.00 30.58           888         O ALA A 234         -18.611         46.555         76.947         1.00 31.37           889         N THR A 235         -16.815         47.389         78.028         1.00 32.78           891         CB THR A 235         -14.533         47.546         77.129										
879       CB       THR A 233       -18.080       46.242       83.085       1.00       31.41         880       OG1       THR A 233       -17.464       45.953       84.337       1.00       28.31         881       CG2       THR A 233       -19.358       45.267       82.986       1.00       28.26         883       O       THR A 233       -17.783       46.052       80.670       1.00       30.81         883       O       THR A 233       -17.783       46.052       80.670       1.00       30.81         884       N       ALA A 234       -18.283       47.261       80.402       1.00       30.12         885       CA       ALA A 234       -18.959       47.533       79.118       1.00       30.91         886       CB       ALA A 234       -18.104       47.102       77.946       1.00       30.58         887       C       ALA A 234       -18.611       46.555       76.947       1.00       31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -14.533       47.546       77.006 <td< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></td<>										
880       OG1       THR A 233       -17.464       45.953       84.337       1.00       28.31         881       CG2       THR A 233       -19.358       45.267       82.986       1.00       28.26         882       C       THR A 233       -17.783       46.052       80.670       1.00       30.81         884       N       ALA A 234       -18.283       47.261       80.402       1.00       30.12         885       CA       ALA A 234       -18.959       47.533       79.118       1.00       30.51         886       CB       ALA A 234       -19.319       48.998       78.963       1.00       29.68         887       C       ALA A 234       -18.104       47.102       77.946       1.00       30.58         888       O       ALA A 234       -18.611       46.555       76.947       1.00       31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -14.654       48.951       77.129       1.00       32.75         891       CB       THR A 235       -13.580       47.153       75.656 <td< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></td<>										
881       CG2       THR A 233       -19.358       45.267       82.986       1.00       28.26         882       C       THR A 233       -17.783       46.052       80.670       1.00       30.81         883       O       THR A 233       -17.937       45.050       79.937       1.00       29.48         884       N       ALA A 234       -18.283       47.261       80.402       1.00       30.12         886       CB       ALA A 234       -18.959       47.533       79.118       1.00       30.91         886       CB       ALA A 234       -18.914       48.998       78.963       1.00       30.58         887       C       ALA A 234       -18.611       46.555       76.947       1.00       30.58         888       O       ALA A 234       -18.611       46.555       76.947       1.00       31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -14.654       48.951       77.006       1.00       34.77         891       CB       THR A 235       -15.860       45.400       76.799       1										
882         C         THR A 233         -17.783         46.052         80.670         1.00         30.81           883         O         THR A 233         -17.937         45.050         79.937         1.00         29.48           884         N         ALA A 234         -18.283         47.261         80.402         1.00         30.12           885         CA         ALA A 234         -18.959         47.533         79.118         1.00         30.91           886         CB         ALA A 234         -19.319         48.998         78.963         1.00         29.68           887         C         ALA A 234         -18.104         47.102         77.946         1.00         30.58           888         O         ALA A 234         -18.611         46.555         76.947         1.00         31.37           889         N         THR A 235         -16.815         47.389         78.028         1.00         30.80           890         CA         THR A 235         -14.654         48.951         77.106         1.00         34.77           891         CB         THR A 235         -13.580         47.153         75.967         1.00         34.42										
883         O         THR A 233         -17.937         45.050         79.937         1.00         29.48           884         N         ALA A 234         -18.283         47.261         80.402         1.00         30.12           885         CA         ALA A 234         -18.959         47.533         79.118         1.00         30.91           886         CB         ALA A 234         -19.319         48.998         78.963         1.00         29.68           887         C         ALA A 234         -18.104         47.102         77.946         1.00         30.58           888         O         ALA A 234         -18.611         46.555         76.947         1.00         31.37           889         N         THR A 235         -16.815         47.389         78.028         1.00         30.80           890         CA         THR A 235         -14.533         47.546         77.129         1.00         32.35           891         CB         THR A 235         -14.654         48.951         77.006         1.00         34.77           893         CG2         THR A 235         -15.860         45.400         76.799         1.00         32.27 <td></td>										
884       N       ALA A 234       -18.283       47.261       80.402       1.00       30.12         885       CA       ALA A 234       -18.959       47.533       79.118       1.00       30.91         886       CB       ALA A 234       -19.319       48.998       78.963       1.00       29.68         887       C       ALA A 234       -18.104       47.102       77.946       1.00       30.58         888       O       ALA A 234       -18.611       46.555       76.947       1.00       31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -15.928       46.948       76.953       1.00       32.35         891       CB       THR A 235       -14.533       47.546       77.129       1.00       32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00       34.77         893       CG2       THR A 235       -15.860       45.400       76.799       1.00       32.27         894       C       THR A 236       -15.711       44.693       77.914 <td< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></td<>										
885       CA       ALA A 234       -18.959       47.533       79.118       1.00 30.91         886       CB       ALA A 234       -19.319       48.998       78.963       1.00 29.68         887       C       ALA A 234       -18.104       47.102       77.946       1.00 30.58         888       O       ALA A 234       -18.611       46.555       76.947       1.00 30.80         890       CA       THR A 235       -16.815       47.389       78.028       1.00 30.80         891       CB       THR A 235       -15.928       46.948       76.953       1.00 32.78         891       CB       THR A 235       -14.533       47.546       77.129       1.00 32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00 34.77         893       CG2       THR A 235       -15.860       45.400       76.799       1.00 32.27         894       C       THR A 235       -16.000       44.850       75.656       1.00 31.74         895       O       THR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.384       42.639										
886       CB       ALA A 234       -19.319       48.998       78.963       1.00 29.68         887       C       ALA A 234       -18.104       47.102       77.946       1.00 30.58         888       O       ALA A 234       -18.611       46.555       76.947       1.00 31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00 30.80         890       CA       THR A 235       -15.928       46.948       76.953       1.00 32.35         891       CB       THR A 235       -14.533       47.546       77.129       1.00 32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00 34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00 34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00 32.27         895       O       THR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.384       42.639       <										
887         C         ALA A 234         -18.104         47.102         77.946         1.00 30.58           888         O         ALA A 234         -18.611         46.555         76.947         1.00 30.80           890         N         THR A 235         -16.815         47.389         78.028         1.00 30.80           890         CA         THR A 235         -15.928         46.948         76.953         1.00 32.35           891         CB         THR A 235         -14.533         47.546         77.129         1.00 32.78           892         OG1         THR A 235         -14.654         48.951         77.006         1.00 34.77           893         CG2         THR A 235         -13.580         47.153         75.967         1.00 34.42           894         C         THR A 235         -15.860         45.400         76.799         1.00 32.27           895         O         THR A 236         -15.711         44.693         77.914         1.00 30.81           897         CA         TYR A 236         -15.676         43.199         77.861         1.00 29.77           898         CB         TYR A 236         -15.384         42.639         79.250         1.00										
888       O       ALA A 234       -18.611       46.555       76.947       1.00       31.37         889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -15.928       46.948       76.953       1.00       32.35         891       CB       THR A 235       -14.533       47.546       77.129       1.00       32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00       34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00       34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00       32.27         895       O       THR A 235       -16.000       44.850       75.656       1.00       31.74         896       N       TYR A 236       -15.676       43.199       77.861       1.00       29.77         898       CB       TYR A 236       -15.384       42.639       79.250       1.00       32.58         900       CD1       TYR A 236       -12.913       42.926       78.818 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
889       N       THR A 235       -16.815       47.389       78.028       1.00       30.80         890       CA       THR A 235       -15.928       46.948       76.953       1.00       32.35         891       CB       THR A 235       -14.533       47.546       77.129       1.00       32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00       34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00       34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00       32.27         895       O       THR A 235       -16.000       44.850       75.656       1.00       31.74         896       N       TYR A 236       -15.711       44.693       77.914       1.00       30.81         897       CA       TYR A 236       -15.384       42.639       79.250       1.00       29.77         898       CB       TYR A 236       -13.950       42.738       79.720       1.00       32.58         901       CE1       TYR A 236       -11.617       42.996       79.243       <										
890       CA       THR A 235       -15.928       46.948       76.953       1.00 32.35         891       CB       THR A 235       -14.533       47.546       77.129       1.00 32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00 34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00 34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00 32.27         895       O       THR A 235       -16.000       44.850       75.656       1.00 31.74         896       N       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.676       43.199       77.861       1.00 29.80         899       CG       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -12.913       42.926       78.818       1.00 32.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.617       42.971										
891       CB       THR A 235       -14.533       47.546       77.129       1.00 32.78         892       OG1       THR A 235       -14.654       48.951       77.006       1.00 34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00 34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00 32.27         895       O       THR A 235       -16.000       44.850       75.656       1.00 31.74         896       N       TYR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1       TYR A 236       -11.617       42.926       78.818       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -12.330       42.686										
892       OG1       THR A 235       -14.654       48.951       77.006       1.00 34.77         893       CG2       THR A 235       -13.580       47.153       75.967       1.00 34.42         894       C THR A 235       -15.860       45.400       76.799       1.00 32.27         895       O THR A 235       -16.000       44.850       75.656       1.00 31.74         896       N TYR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1 TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1 TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2 TYR A 236       -13.643       42.62										
893       CG2       THR A 235       -13.580       47.153       75.967       1.00 34.42         894       C       THR A 235       -15.860       45.400       76.799       1.00 32.27         895       O       THR A 235       -16.000       44.850       75.656       1.00 31.74         896       N       TYR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1       TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.628										
894         C         THR A 235         -15.860         45.400         76.799         1.00         32.27           895         O         THR A 235         -16.000         44.850         75.656         1.00         31.74           896         N         TYR A 236         -15.711         44.693         77.914         1.00         30.81           897         CA         TYR A 236         -15.676         43.199         77.861         1.00         29.77           898         CB         TYR A 236         -15.384         42.639         79.250         1.00         29.80           899         CG         TYR A 236         -13.950         42.738         79.720         1.00         32.58           900         CD1         TYR A 236         -12.913         42.926         78.818         1.00         33.58           901         CE1         TYR A 236         -11.617         42.996         79.243         1.00         36.97           902         CZ         TYR A 236         -11.324         42.872         80.601         1.00         36.77           903         OH         TYR A 236         -12.330         42.686         81.516         1.00         35.78     <										
895       O       THR A 235       -16.000       44.850       75.656       1.00 31.74         896       N       TYR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1       TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680										
896       N       TYR A 236       -15.711       44.693       77.914       1.00 30.81         897       CA       TYR A 236       -15.676       43.199       77.861       1.00 29.77         898       CB       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1       TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680										
897         CA         TYR A 236         -15.676         43.199         77.861         1.00 29.77           898         CB         TYR A 236         -15.384         42.639         79.250         1.00 29.80           899         CG         TYR A 236         -13.950         42.738         79.720         1.00 32.58           900         CD1         TYR A 236         -12.913         42.926         78.818         1.00 35.58           901         CE1         TYR A 236         -11.617         42.996         79.243         1.00 36.97           902         CZ         TYR A 236         -11.324         42.872         80.601         1.00 36.77           903         OH         TYR A 236         -10.025         42.971         81.016         1.00 37.51           904         CE2         TYR A 236         -12.330         42.686         81.516         1.00 35.78           905         CD2         TYR A 236         -13.643         42.634         81.065         1.00 36.22           906         C         TYR A 236         -17.042         42.628         77.377         1.00 29.01           907         O         TYR A 236         -17.103         41.680         76.632										
898       CB       TYR A 236       -15.384       42.639       79.250       1.00 29.80         899       CG       TYR A 236       -13.950       42.738       79.720       1.00 32.58         900       CD1       TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00 29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00 30.01										
899       CG       TYR A 236       -13.950       42.738       79.720       1.00       32.58         900       CD1       TYR A 236       -12.913       42.926       78.818       1.00       33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00       36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00       36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00       37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00       35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00       36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00       29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00       29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00       30.01										
900       CD1       TYR A 236       -12.913       42.926       78.818       1.00 33.58         901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00 29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00 30.01										
901       CE1       TYR A 236       -11.617       42.996       79.243       1.00 36.97         902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00 29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00 30.01										
902       CZ       TYR A 236       -11.324       42.872       80.601       1.00 36.77         903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00 29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00 30.01										
903       OH       TYR A 236       -10.025       42.971       81.016       1.00 37.51         904       CE2       TYR A 236       -12.330       42.686       81.516       1.00 35.78         905       CD2       TYR A 236       -13.643       42.634       81.065       1.00 36.22         906       C       TYR A 236       -17.042       42.628       77.377       1.00 29.01         907       O       TYR A 236       -17.103       41.680       76.632       1.00 29.48         908       N       ILE A 237       -18.139       43.236       77.814       1.00 30.01										
904 CE2 TYR A 236										
905 CD2 TYR A 236										
906 C TYR A 236 -17.042 42.628 77.377 1.00 29.01 907 O TYR A 236 -17.103 41.680 76.632 1.00 29.48 908 N ILE A 237 -18.139 43.236 77.814 1.00 30.01										
907 O TYR A 236 -17.103 41.680 76.632 1.00 29.48 908 N ILE A 237 -18.139 43.236 77.814 1.00 30.01										
908 N ILE A 237 -18.139 43.236 77.814 1.00 30.01										

### FIGURE 3R

A	В	С	D	E		F	G		Н	I	J
910	СВ	ILE	Α	237	-2(	).591	43.548	7	8.061	1.00	29.26
911	CG1			237		580	43.141		9.541		31.33
912	CD1	ILE	Α	237	-20	0.607	41.494	7	9.786	1.00	32.72
913	CG2	ILE	Α	237	-23	1.938	43.089	7	7.553	1.00	30.76
914	С	ILE	Α	237	-19	9.524	42.975	7	5.874	1.00	30.97
915	0	ILE	Α	237	-20	0.024	42.110	7	5.165	1.00	28.59
916	N	THR	Α	238	-19	9.071	44.126	7	5.413	1.00	29.66
917	CA	THR	Α	238	-19	9.074	44.331	7	3.936	1.00	31.58
918	CB	THR	Α	238	-18	3.483	45.699	7	3.600	1.00	30.71
919	OG1	THR	Α	238	-19	9.345	46.681		4.169		33.26
920	CG2			238	-18	3.547	45.948	7	2.092	1.00	36.01
921	С			238		3.279	43.281		3.177		31.08
922	0			238		3.744	42.785	7.	2.179	1.00	31.90
923	N	GLU	Α	239		7.037	43.029	7	3.578		30.93
924	CA	GLU	Α	239	-16	5.252	41.972	7.	2.973		33.24
925	CB	GLU	Α	239		1.875	41.829		3.619	1.00	
926	CG			239		1.045	43.126		3.458		41.57
927	CD			239		2.704	43.109		4.200	1.00	
928	OE1			239		1.654	43.089		3.518		59.72
929	OE2	GLU				2.655	43.120		5.451		51.19
930	С			239		5.947	40.625		2.977		32.47
931	0			239		5.890	39.912		2.000		31.96
932	Ν			240		7.585	40.307		4.093		31.66
933	CA			240		3.252	39.033		4.293		32.00
934	СВ			240		3.793	38.941		5.749		32.28
935	CG			240		7.918	38.368		6.879	1.00	
936	CD1			240		7.987	39.156		8.226		40.94
937	CD2			240		3.427	36.978		7.180		46.36
938	С			240		9.433	38.992		3.363		31.20
939	0			240		9.674	37.997		2.730		30.06
940	N	ALA				1.189	40.074		3.311		30.48
941 942	CA CB	ALA		241		L.385	40.079 41.336		2.470 2.673		30.85
942	СБ			241		2.161 1.046	39.875		0.996		28.64 32.63
944	0			241		1.803	39.233		0.268		34.13
945	N			241		9.946	40.476		0.200		32.98
946	CA	ASN				9.501	40.301		9.176		34.79
947	CB			242			41.225		8.806		35.05
948	CG			242		3.735	42.668		8.801		37.46
949	OD1	ASN				9.820	43.009		8.356		41.91
950	ND2	ASN				7.838	43.531		9.270		36.72
951	C			242		9.045	38.878		8.944		33.66
952	0			242		9.384	38.322		7.926		34.14
953	N			243		3.284	38.287		9.871		33.13
954	CA			243		7.846	36.899		9.686		33.50
955	СВ			243		5.883	36.413		0.821		32.46
956	C			243		9.100	36.026		9.596		33.00
957	0			243		9.170	35.121		8.775		34.04
958	N			244		0.063	36.281		0.460		32.30
959	CA			244		1.290	35.495		0.486		34.17
960	СВ			244		2.109	35.794		1.761		32.72

### FIGURE 3S

А	В	С	D	E	F	G	Н	I	J
961	CG	LEU	Α	244	-21.487	35.248	73.091	1.00	33.90
962	CD1	LEU			-22.375	35.636	74.211	1.00	34.58
963	CD2	LEU			-21.346	33.731	73.053	1.00	36.04
964	С	LEU		244	-22.155	35.710	69.239	1.00	35.07
965	0	LEU			-22.795	34.770	68.771	1.00	35.54
966	N	SER		245	-22.205	36.935	68.736	1.00	36.14
967	CA			245	-22.968	37.144	67.497	1.00	37.32
968 969	CB OG			<ul><li>245</li><li>245</li></ul>	-22.881 -23.518	38.566 39.430	66.993 67.885	1.00	36.71 40.23
970	C			245	-22.396	36.244	66.430	1.00	37.77
971	0			245	-23.168	35.561	65.712	1.00	39.78
972	N			246	-21.062	36.236	66.324	1.00	36.62
973	CA			246	-20.388	35.397	65.334	1.00	36.75
974	СВ			246	-18.867	35.666	65.303	1.00	35.63
975	CG	TYR	Α	246	-18.040	34.768	64.415	1.00	36.74
976	CD1	TYR	Α	246	-17.752	35.114	63.086	1.00	41.06
977	CE1			246	-16.991	34.283	62.293	1.00	40.63
978	CZ			246	-16.491	33.118	62.824	1.00	42.34
979	ОН			246	-15.711	32.256	62.077	1.00	41.50
980	CE2			246	-16.782	32.766	64.151	1.00	40.05
981	CD2			246	-17.538	33.590	64.897	1.00	34.12
982	С			246	-20.730	33.925	65.554	1.00	36.80
983 984	N			246 247	-21.143	33.248 33.425	64.624 66.778	1.00	36.65
985	CA			247	-20.608 -21.015	32.049	67.085	1.00	36.48 36.90
986	CB			247	-20.803	31.722	68.595	1.00	37.60
987	SG			247	-19.067	31.666	69.093	1.00	42.84
988	C			247	-22.473	31.711	66.758	1.00	37.39
989	0			247	-22.746	30.672	66.121	1.00	37.58
990	N	HIS		248	-23.400	32.529	67.256	1.00	36.67
991	CA	HIS	Α	248	-24.817	32.267	67.094	1.00	37.58
992	CB	HIS		248	-25.698	33.244	67.876	1.00	37.99
993	CG	HIS		248	-25.520	33.191	69.372	1.00	34.73
994	ND1	HIS			-26.053	34.149	70.204	1.00	36.33
995	CE1			248	-25.718	33.886	71.452	1.00	37.79
996	NE2	HIS			-24.957	32.807	71.458	1.00	33.84
997		HIS			-24.812	32.354	70.168	1.00	33.28
998 999	C 0	HIS HIS			-25.189 -26.098	32.338 31.629	65.601 65.132		39.08 39.68
1000	И			249	-24.443	33.132	64.854	1.00	39.67
1001	CA			249	-24.748	33.244	63.437		41.50
1002	СВ			249	-23.805	34.207	62.715		40.00
1003	OG			249	-22.561	33.599	62.481		41.00
1004	С			249	-24.644	31.857	62.870		42.73
1005	0			249	-25.312	31.550	61.894	1.00	43.62
1006	N			250	-23.799	31.026	63.476	1.00	43.39
1007	CA			250	-23.626	29.655	63.026	1.00	44.23
1008	СВ	LYS			-22.163	29.299	63.057	1.00	45.26
1009	CG			250	-21.329	30.154	62.111	1.00	46.88
1010	CD			250	-19.847	29.989	62.369		46.41
1011	CE	ПΙЭ	Н	250	-19.102	31.086	61.674	1.00	50.41

## FIGURE 3T

A	В	С	D	E	F	G	Н	I	J
1012	NZ	TVC	7\	250	-18.101	30.510	60.721	1 00	55.71
1012	C			250	-24.430	28.706	63.912		44.23
1013	0			250	-24.318	27.494	63.813		44.92
1015	N			251	-25.252	29.280	64.771	1.00	
1016	CA			251	-26.013	28.499	65.722	1.00	
1017	CB			251	-27.003	27.566	65.025	1.00	
1017	CG			251	-28.079	28.334	64.298		48.00
1019	CD	ARG			-29.293	28.613	65.135	1.00	52.94
1020	NE			251	-30.316	27.613	64.935	1.00	57.46
1021	CZ			251	-31.409	27.504	65.694	1.00	59.77
1021	NH1	ARG			-32.301	26.573	65.421	1.00	58.50
1023	NH2	ARG			-31.617	28.329	66.721	1.00	
1023	C			251	-25.133	27.719	66.694	1.00	40.87
1025	0			251	-25.579	26.725	67.287	1.00	
1026	N			252	-23.890	28.136	66.866	1.00	
1027	CA	VAL			-23.090	27.469	67.883		
1028	CB	VAL			-21.605	27.579	67.574	1.00	36.71
1029	CG1	VAL			-20.757	27.253	68.833	1.00	36.16
1030	CG2	VAL			-21.267	26.671	66.408	1.00	32.96
1031	C			252	-23.398	28.171	69.217	1.00	35.05
1032	0			252	-23.342	29.421	69.278	1.00	34.28
1033	N			253	-23.751	27.394	70.238	1.00	34.78
1034	CA			253	-24.036	27.990	71.537		34.21
1035	СВ			253	-25.528	27.772	72.035		36.92
1036	CG1	ILE		253	-26.008	26.317	72.080		34.92
1037	CD1	ILE		253	-27.473	26.046	72.506	1.00	33.07
1038	CG2			253	-26.490	28.538	71.085	1.00	39.25
1039	С			253	-22.899	27.570	72.441	1.00	32.53
1040	0			253	-22.459	26.397	72.378	1.00	32.33
1041	N	HIS	Α	254	-22.352	28.508	73.234	1.00	30.81
1042	CA	HIS	Α	254	-21.118	28.158	73.987	1.00	29.80
1043	СВ	HIS	Α	254	-20.268	29.410	74.275	1.00	29.82
1044	CG	HIS	Α	254	-19.012	29.095	75.010	1.00	27.09
1045	ND1	HIS	Α	254	-19.012	28.695	76.327	1.00	28.08
1046	CE1	HIS	Α	254	-17.763	28.515	76.729	1.00	29.12
1047	NE2	HIS	Α	254	-16.960	28.776	75.712	1.00	31.85
1048	CD2	HIS	Α	254	-17.712	29.137	74.622	1.00	26.39
1049	С	HIS	Α	254	-21.449	27.412	75.287	1.00	29.59
1050	0	HIS	Α	254	-20.897	26.345	75.563	1.00	28.85
1051	N	ARG	Α	255	-22.405	27.957	76.024	1.00	30.83
1052	CA	ARG	Α	255	-22.920	27.309	77.234	1.00	30.64
1053	СВ	ARG	Α	255	-23.388	25.859	76.916		30.22
1054	CG	ARG			-24.321	25.716	75.687		32.25
1055	CD	ARG			-25.189	24.432	75.685	1.00	31.75
1056	NE	ARG			-24.362	23.256	75.649	1.00	30.77
1057	CZ	ARG			-24.820	22.017	75.669	1.00	31.35
1058	NH1	ARG			-26.095	21.798	75.751		31.83
1059	NH2	ARG			-23.977	21.003	75.617		33.16
1060	С			255	-21.983	27.279	78.449		31.38
1061	0			255	-22.363	26.734	79.477		32.65
1062	N	ASP	Α	256	-20.758	27.768	78.356	1.00	31.39

## FIGURE 3U

A	В	С	D	Ε	F	G	Н	I	J
1063	CA	ASP	Α	256	-19.870	27.725	79.524	1.00	31.75
1064	СВ			256	-18.964	26.468	79.453		33.11
1065	CG			256	-18.280	26.139	80.746	1.00	35.07
1066		ASP			-18.773	26.510	81.850	1.00	
1067		ASP			-17.221	25.488	80.765	1.00	36.02
1068	C			256	-19.086	29.003	79.566	1.00	31.14
1069	0			256	-17.867	29.025	79.770	1.00	30.07
1070	И			257	-19.785	30.091	79.314	1.00	
1071	CA			257	-19.166	31.390	79.385	1.00	32.07
1071	CB			257	-20.057	32.311	78.676	1.00	32.32
1072	CG1	ILE			-19.935	31.982	77.143	1.00	33.96
1073	CD1	ILE			-21.111	32.476	76.377	1.00	
1074	CG2			257	-19.737	33.701	78.956	1.00	34.18
1075	C			257	-19.064	31.704	80.897	1.00	33.31
1077	0			257	-20.100	31.754	81.616	1.00	
1077	N			258	-17.824	31.761	81.371	1.00	31.48
1078	CA			258	-17.524	32.187	82.750	1.00	30.84
1079	CB			258	-17.738	31.082	83.740	1.00	30.14
1081	CG			258	-16.926	29.870	83.529	1.00	34.40
1081	CD			258	-17.629	28.644	84.283	1.00	38.03
1083	CE			258	-16.742	27.431	84.270	1.00	41.53
1083	NZ			258	-17.580	26.165	84.236	1.00	42.89
1085	C			258	-16.097	32.737	82.755	1.00	30.04
1086	0			258	-15.324	32.737	81.785	1.00	
1087	И			259	-15.775	33.505	83.792	1.00	28.33
1088	CA			259	-14.498	34.201	83.824	1.00	28.63
1089	CB			259	-14.480	34.892	85.200		27.18
1090	CG			259	-15.974	35.164	85.421		28.54
1091	CD			259	-16.648	33.843	84.942		29.43
1092	C			259	-13.330	33.301	83.615	1.00	27.22
1093	0			259	-12.411	33.740	82.963	1.00	
1094	N			260	-13.331	32.086	84.121	1.00	
1095	CA			260	-12.176	31.226	83.876		28.92
1096	СВ			260	-12.107	30.028	84.836		31.10
1097	CG			260	-13.445	29.310	84.935	1.00	35.20
1098	CD			260	-14.340	29.861	86.098	1.00	44.01
1099	OE1	GLU	Α	260	-14.462	29.148	87.133	1.00	
1100		GLU			-14.908	30.985			33.54
1101	С			260	-12.027	30.755	82.420		28.10
1102	0			260	-10.957	30.265	82.068		29.64
1103	N	ASN	Α	261	-13.012	30.991	81.567		26.88
1104	CA			261	-12.871	30.603	80.189		26.98
1105	СВ			261	-14.077	29.731	79.753	1.00	26.91
1106	CG	ASN	Α	261	-14.099	28.389	80.436		26.82
1107		ASN			-13.048	27.832	80.771		28.36
1108		ASN			-15.322	27.808	80.578	1.00	25.54
1109	С	ASN	Α	261	-12.786	31.829	79.266	1.00	28.17
1110	0	ASN	Α	261	-12.988	31.685	78.040		28.42
1111	N	LEU	Α	262	-12.540	33.021	79.848		27.97
1112	CA			262	-12.454	34.254	79.091		28.33
1113	СВ	LEU	Α	262	-13.351	35.341	79.662	1.00	29.50

#### FIGURE 3V

A	В	С	D	E	F	G	Н	I	J
1114	CG	LEU	А	262	-14.856	35.024	79.655	1.00	28.47
1115	CD1	LEU	Α	262	-15.646	36.167	80.215	1.00	30.27
1116	CD2	LEU	Α	262	-15.308	34.782	78.142	1.00	27.13
1117	С	LEU	Α	262	-11.011	34.681	79.268	1.00	29.16
1118	0			262	-10.554	34.891	80.405	1.00	28.97
1119	N			263	-10.299	34.765	78.163	1.00	26.56
1120	CA			263	-8.869	34.988	78.194	1.00	28.18
1121	СВ			263	-8.103	33.942	77.360	1.00	
1122	CG			263	-8.452	32.452	77.583	1.00	
1123	CD1			263	-7.487	31.481	76.825	1.00	30.33
1124	CD2	LEU			-8.272	32.171	79.060	1.00	34.69
1125	C			263	-8.574	36.382	77.619		29.97
1126	0			263	-9.416	37.002	76.966		29.84
1127	N			264	-7.378	36.850	77.904	1.00	30.85
1128	CA			264	-6.951	38.182	77.486	1.00	30.74
1129	СВ			264	-6.721	39.079	78.732	1.00	30.19
1130	CG			264	-7.965	39.287	79.626	1.00	
1131	CD1			264	-7.590	39.909	81.031	1.00	
1132	CD2	LEU			-9.105	40.109	78.954	1.00	31.52
1133	C			264	-5.737	38.121	76.554	1.00	30.62
1134	0			264	-4.722	37.498	76.853		29.43
1135	N	GLY			-5.901	38.736	75.390	1.00	31.75
1136	CA			265	-4.858	38.816	74.396	1.00	33.01
1137	С			265	-3.830	39.883	74.737	1.00	34.94
1138	0	GLY	Α	265	-3.969	40.574	75.751	1.00	34.96
1139	N	SER	Α	266	-2.807	40.035	73.891	1.00	36.48
1140	CA	SER	Α	266	-1.722	40.978	74.178	1.00	39.30
1141	СВ	SER	Α	266	-0.547	40.820	73.179	1.00	39.61
1142	OG	SER	Α	266	-1.009	40.865	71.841	1.00	45.24
1143	С	SER	Α	266	-2.195	42.443	74.287	1.00	39.68
1144	0	SER	Α	266	-1.591	43.221	74.989	1.00	41.74
1145	N	ALA	Α	267	-3.286	42.827	73.641	1.00	39.84
1146	CA	ALA	Α	267	-3.757	44.193	73.821	1.00	40.82
1147	СВ	ALA	Α	267	-4.312	44.745	72.510	1.00	41.57
1148	С	ALA	Α	267	-4.826	44.245	74.881	1.00	40.28
1149	0			267	-5.507	45.246	75.017	1.00	
1150	Ν	GLY			-4.999	43.160	75.616	1.00	38.92
1151	CA	GLY				43.099			39.91
1152	С			268	-7.440	42.772	76.035		39.16
1153	0			268	-8.421	42.894	76.749		39.70
1154	Ν			269	-7.525	42.328	74.781		37.55
1155	CA			269	-8.846	42.066	74.210		37.18
1156	СВ			269	-8.844	42.024	72.686	1.00	
1157	CG			269	-7.914	40.966	72.111		42.45
1158	CD OF 1			269	-6.497	41.495	71.931		48.18
1159	OE1	GLU			-5.789	41.696	72.951		49.56
1160					-6.122	41.758	70.767		54.50
1161 1162	С			269	-9.323 -8.556	40.711	74.736	1.00	
	O N			269	-8.556	39.821 40.599	74.981		32.16 33.25
1163 1164	N CA			<ul><li>270</li><li>270</li></ul>	-10.611	39.438	74.889 75.496		33.59
T T O 4	CA	∪ن∟	Д	2/0	11.100	JJ.430	10.400	1.00	55.55

### FIGURE 3W

1165	A	В	С	D	Ε	F	G	Н	I	J
1166	1165	CD.	T 1711	71	270	10 E20	20 026	76 065	1 00	22 76
1167   CD1   LEU A 270										
1168										
1169										
1170										
1171 N LYS A 271										
1172 CA LYS A 271										
1173										
1174										
1175   CD										
1176										
1177   NZ										
1178										
1179										
1180         N         ILE A 272         -13.062         34.408         73.997         1.00         29.63           1181         CA         ILE A 272         -13.770         33.287         74.572         1.00         31.28           1182         CB         ILE A 272         -15.251         33.238         74.154         1.00         32.97           1183         CGI         ILE A 272         -15.867         31.943         74.660         1.00         34.14           1184         CDI         ILE A 272         -15.415         33.105         72.693         1.00         36.72           1185         CG2         ILE A 272         -12.981         32.023         74.227         1.00         29.77           1187         O         ILE A 272         -12.881         33.105         72.693         1.00         29.77           1187         O         ILE A 272         -12.981         33.105         72.693         1.00         29.77           1187         O         ILE A 272         -12.981         33.105         75.040         1.00         29.03           1188         CA         ALA A 273         -12.072         29.905         75.040         1.00         28.02<										
1181         CA         ILE A 272         -13.770         33.287         74.572         1.00         31.28           1182         CB         ILE A 272         -15.251         33.238         74.154         1.00         32.97           1183         CG1         ILE A 272         -15.867         31.943         74.660         1.00         34.14           1184         CD1         ILE A 272         -15.415         33.105         72.693         1.00         36.72           1186         C         ILE A 272         -12.981         32.023         74.227         1.00         29.77           1187         O         ILE A 272         -12.487         31.888         73.131         1.00         29.32           1188         N         ALA A 273         -12.072         29.905         75.040         1.00         29.93           1190         CB         ALA A 273         -12.890         28.757         75.639         1.00         28.29           1191         C         ALA A 273         -14.008         28.975         75.639         1.00         28.29           1192         O         ALA A 273         -14.008         28.975         75.639         1.00         28.29 <td></td>										
1182         CB         ILE A 272         -15.251         33.238         74.154         1.00 32.97           1183         CG1         ILE A 272         -15.867         31.943         74.660         1.00 34.14           1184         CD1         ILE A 272         -17.133         32.166         75.428         1.00 41.15           1185         CG2         ILE A 272         -12.981         32.023         74.227         1.00 29.77           1187         O         ILE A 272         -12.487         31.888         73.131         1.00 29.32           1188         N         ALA A 273         -12.833         31.121         75.199         1.00 29.03           1189         CA         ALA A 273         -12.072         29.905         75.040         1.00 28.02           1190         CB         ALA A 273         -12.890         28.757         75.696         1.00 28.47           1191         C         ALA A 273         -14.008         28.975         76.165         1.00 29.27           1193         N         ASP A 274         -12.329         27.558         75.567         1.00 28.32           1194         CA         ASP A 274         -13.273         25.239         78.444										
1183										
1184 CD1 ILE A 272										
1185         CG2         ILE A 272         -15.415         33.105         72.693         1.00 36.72           1186         C         ILE A 272         -12.981         32.023         74.227         1.00 29.77           1187         O         ILE A 272         -12.487         31.888         73.131         1.00 29.03           1189         CA         ALA A 273         -12.833         31.121         75.199         1.00 29.03           1189         CA         ALA A 273         -12.072         29.905         75.040         1.00 25.93           1190         CB         ALA A 273         -10.720         30.027         75.796         1.00 25.93           1191         C         ALA A 273         -12.890         28.757         75.639         1.00 28.47           1192         O         ALA A 273         -14.008         28.975         76.165         1.00 29.27           1193         N         ASP A 274         -12.329         27.558         75.567         1.00 30.13           1195         CB         ASP A 274         -12.990         26.361         76.217         1.00 30.13           1195         CB         ASP A 274         -12.994         26.548         77.752										
1186         C         ILE A 272         -12.981         32.023         74.227         1.00 29.77           1187         O         ILE A 272         -12.487         31.888         73.131         1.00 29.32           1188         N         ALA A 273         -12.833         31.121         75.199         1.00 29.03           1189         CA         ALA A 273         -12.072         29.905         75.040         1.00 25.93           1190         CB         ALA A 273         -10.720         30.027         75.796         1.00 28.47           1192         O         ALA A 273         -12.890         28.757         75.639         1.00 28.32           1193         N         ASP A 274         -12.329         27.558         75.567         1.00 28.32           1194         CA         ASP A 274         -12.329         27.558         75.567         1.00 28.32           1194         CA         ASP A 274         -12.990         26.361         76.217         1.00 30.13           1195         CB         ASP A 274         -13.273         25.239         78.444         1.00 30.13           1197         OD1         ASP A 274         -13.354         25.219         79.681										
1187         O         ILE A 272         -12.487         31.888         73.131         1.00 29.32           1188         N         ALA A 273         -12.833         31.121         75.199         1.00 29.03           1189         CA         ALA A 273         -12.072         29.905         75.040         1.00 28.02           1190         CB         ALA A 273         -10.720         30.027         75.796         1.00 29.27           1191         C         ALA A 273         -14.008         28.757         75.639         1.00 29.27           1193         N         ASP A 274         -12.329         27.558         75.567         1.00 28.32           1194         CA         ASP A 274         -12.329         27.558         75.567         1.00 28.19           1195         CB         ASP A 274         -12.994         26.548         77.752         1.00 28.19           1196         CG         ASP A 274         -13.273         25.239         78.444         1.00 30.13           1197         OD1         ASP A 274         -13.354         25.219         79.681         1.00 27.79           1198         OD2         ASP A 274         -13.407         24.145         77.794										
1188         N         ALA A 273         -12.833         31.121         75.199         1.00         29.03           1189         CA         ALA A 273         -12.072         29.905         75.040         1.00         28.02           1190         CB         ALA A 273         -10.720         30.027         75.796         1.00         25.93           1191         C         ALA A 273         -12.890         28.757         75.639         1.00         28.47           1192         O         ALA A 273         -14.008         28.975         75.567         1.00         29.27           1193         N         ASP A 274         -12.329         27.558         75.567         1.00         28.32           1194         CA         ASP A 274         -12.990         26.361         76.217         1.00         28.19           1195         CB         ASP A 274         -12.994         26.548         77.752         1.00         28.19           1196         CG         ASP A 274         -13.273         25.239         78.444         1.00         30.91           1197         OD1         ASP A 274         -13.407         24.145         77.794         1.00         32.55 <td></td>										
1189       CA       ALA A 273       -12.072       29.905       75.040       1.00       28.02         1190       CB       ALA A 273       -10.720       30.027       75.796       1.00       25.93         1191       C       ALA A 273       -12.890       28.757       75.639       1.00       28.47         1192       O       ALA A 273       -14.008       28.975       76.165       1.00       29.27         1193       N       ASP A 274       -12.329       27.558       75.567       1.00       28.32         1194       CA       ASP A 274       -12.990       26.361       76.217       1.00       30.13         1195       CB       ASP A 274       -12.994       26.548       77.752       1.00       28.19         1196       CG       ASP A 274       -13.273       25.239       78.444       1.00       30.91         1197       OD1       ASP A 274       -13.407       24.145       77.794       1.00       33.55         1199       C       ASP A 274       -14.278       25.977       75.649       1.00       29.79         1201       N       PHE A 275       -14.288       25.489       74.427										
1190 CB ALA A 273										
1191 C ALA A 273										
1192       O       ALA A 273       -14.008       28.975       76.165       1.00 29.27         1193       N       ASP A 274       -12.329       27.558       75.567       1.00 28.32         1194       CA       ASP A 274       -12.900       26.361       76.217       1.00 30.13         1195       CB       ASP A 274       -12.994       26.548       77.752       1.00 28.19         1196       CG       ASP A 274       -13.273       25.239       78.444       1.00 30.91         1197       OD1       ASP A 274       -13.354       25.219       79.681       1.00 27.79         1198       OD2       ASP A 274       -13.407       24.145       77.794       1.00 33.55         1199       C       ASP A 274       -14.278       25.977       75.649       1.00 29.52         1200       O       ASP A 274       -15.326       26.170       76.275       1.00 28.76         1201       N       PHE A 275       -14.288       25.489       74.427       1.00 29.79         1202       CA       PHE A 275       -15.564       25.206       73.796       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887<										
1193 N ASP A 274										
1194       CA       ASP A 274       -12.900       26.361       76.217       1.00       30.13         1195       CB       ASP A 274       -12.994       26.548       77.752       1.00       28.19         1196       CG       ASP A 274       -13.273       25.239       78.444       1.00       30.91         1197       OD1       ASP A 274       -13.354       25.219       79.681       1.00       27.79         1198       OD2       ASP A 274       -13.407       24.145       77.794       1.00       33.55         1199       C       ASP A 274       -14.278       25.977       75.649       1.00       29.52         1200       O       ASP A 274       -14.278       25.977       75.649       1.00       29.52         1201       N       PHE A 275       -14.288       25.477       76.275       1.00       28.76         1201       N       PHE A 275       -15.564       25.206       73.796       1.00       31.48         1203       CB       PHE A 275       -15.621       26.887       71.890       1.00       30.13         1204       CG       PHE A 275       -14.605       27.761       72.243 <td></td>										
1195         CB         ASP A 274         -12.994         26.548         77.752         1.00 28.19           1196         CG         ASP A 274         -13.273         25.239         78.444         1.00 30.91           1197         OD1 ASP A 274         -13.354         25.219         79.681         1.00 27.79           1198         OD2 ASP A 274         -13.407         24.145         77.794         1.00 33.55           1199         C ASP A 274         -14.278         25.977         75.649         1.00 29.52           1200         O ASP A 274         -15.326         26.170         76.275         1.00 28.76           1201         N PHE A 275         -14.288         25.489         74.427         1.00 29.79           1202         CA PHE A 275         -15.564         25.206         73.796         1.00 31.48           1203         CB PHE A 275         -15.508         25.464         72.250         1.00 30.13           1204         CG PHE A 275         -15.621         26.887         71.890         1.00 30.82           1205         CD1 PHE A 275         -14.605         27.761         72.243         1.00 30.66           1207         CZ PHE A 275         -16.846         28.718										
1196 CG ASP A 274										
1197 OD1 ASP A 274										
1198 OD2 ASP A 274										
1199       C       ASP A 274       -14.278       25.977       75.649       1.00 29.52         1200       O       ASP A 274       -15.326       26.170       76.275       1.00 28.76         1201       N       PHE A 275       -14.288       25.489       74.427       1.00 29.79         1202       CA       PHE A 275       -15.564       25.206       73.796       1.00 31.48         1203       CB       PHE A 275       -15.508       25.464       72.250       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333										
1200       O       ASP A 274       -15.326       26.170       76.275       1.00 28.76         1201       N       PHE A 275       -14.288       25.489       74.427       1.00 29.79         1202       CA       PHE A 275       -15.564       25.206       73.796       1.00 31.48         1203       CB       PHE A 275       -15.508       25.464       72.250       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.1										
1201       N       PHE A 275       -14.288       25.489       74.427       1.00 29.79         1202       CA       PHE A 275       -15.564       25.206       73.796       1.00 31.48         1203       CB       PHE A 275       -15.508       25.464       72.250       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 32.57         1213       CA       GLY A 276       -15.542       23.										
1202       CA       PHE A 275       -15.564       25.206       73.796       1.00 31.48         1203       CB       PHE A 275       -15.508       25.464       72.250       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.										
1203       CB       PHE A 275       -15.508       25.464       72.250       1.00 30.13         1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63										
1204       CG       PHE A 275       -15.621       26.887       71.890       1.00 30.02         1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1205       CD1       PHE A 275       -14.605       27.761       72.243       1.00 30.82         1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63										
1206       CE1       PHE A 275       -14.705       29.121       71.908       1.00 31.65         1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1207       CZ       PHE A 275       -15.847       29.599       71.217       1.00 30.66         1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1208       CE2       PHE A 275       -16.846       28.718       70.853       1.00 28.29         1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.63         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1209       CD2       PHE A 275       -16.707       27.356       71.175       1.00 28.74         1210       C       PHE A 275       -16.042       23.793       74.019       1.00 31.32         1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.27         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1210     C     PHE A 275     -16.042     23.793     74.019     1.00 31.32       1211     O     PHE A 275     -16.874     23.333     73.263     1.00 33.58       1212     N     GLY A 276     -15.542     23.128     75.050     1.00 32.57       1213     CA     GLY A 276     -15.980     21.764     75.409     1.00 33.27       1214     C     GLY A 276     -17.470     21.591     75.718     1.00 33.63										
1211       O       PHE A 275       -16.874       23.333       73.263       1.00 33.58         1212       N       GLY A 276       -15.542       23.128       75.050       1.00 32.57         1213       CA       GLY A 276       -15.980       21.764       75.409       1.00 33.27         1214       C       GLY A 276       -17.470       21.591       75.718       1.00 33.63										
1212 N GLY A 276 -15.542 23.128 75.050 1.00 32.57 1213 CA GLY A 276 -15.980 21.764 75.409 1.00 33.27 1214 C GLY A 276 -17.470 21.591 75.718 1.00 33.63										
1213 CA GLY A 276 -15.980 21.764 75.409 1.00 33.27 1214 C GLY A 276 -17.470 21.591 75.718 1.00 33.63										
1214 C GLY A 276 -17.470 21.591 75.718 1.00 33.63										

#### FIGURE 3X

A	В	С	D	E	F	G	Н	I	J
1216	N	TRP	Α	277	-18.168	22.649	76.085	1.00	32.48
1217	CA	TRP	Α	277	-19.590	22.515	76.352	1.00	32.61
1218	СВ	TRP	Α	277	-19.996	23.356	77.571	1.00	31.90
1219	CG			277	-19.872	22.560	78.827	1.00	
1220	CD1	TRP	Α	277	-18.906	22.655	79.755		35.79
1221	NE1			277	-19.139	21.779	80.781	1.00	39.83
1222	CE2			277	-20.287	21.083	80.520	1.00	
1223	CD2			277	-20.784	21.563	79.295		36.18
1224	CE3			277	-21.976	21.021	78.795		37.42
1225	CZ3			277	-22.625	19.991	79.531		40.23
1226	CH2			277	-22.103	19.550	80.772	1.00	
1227	CZ2			277	-20.945	20.080	81.281	1.00	
1228	С			277	-20.375	22.965	75.141	1.00	
1229	0			277	-21.575	22.921	75.138		31.92
1230	N			278	-19.701	23.425	74.102	1.00	
1231	CA			278	-20.489	23.978	73.041		32.01
1232	СВ			278	-19.643	24.889	72.181		32.28
1233	OG			278	-18.600	24.165	71.545		37.30
1234	С			278	-21.253	22.892	72.194		33.25
1235	0			278	-20.861	21.734	72.149	1.00	
1236	N			279	-22.353	23.307	71.560	1.00	34.55
1237	CA			279	-23.201	22.424	70.775	1.00	
1238	СВ			279	-24.238	21.763	71.710	1.00	
1239	CG1			279	-25.173	22.788	72.273	1.00	
1240	CG2	VAL			-24.920	20.585	71.018	1.00	
1241	С	VAL	Α	279	-23.873	23.260	69.702	1.00	36.61
1242	0	VAL	Α	279	-23.927	24.488	69.850	1.00	35.60
1243	N	HIS	Α	280	-24.438	22.679	68.636	1.00	37.41
1244	CA	HIS	Α	280	-25.231	23.526	67.764	1.00	37.57
1245	CB	HIS	Α	280	-25.245	22.996	66.333	1.00	39.08
1246	CG	HIS	Α	280	-23.897	23.025	65.714	1.00	39.44
1247	ND1	HIS	Α	280	-23.001	21.988	65.841	1.00	45.81
1248	CE1	HIS	Α	280	-21.883	22.296	65.203	1.00	45.95
1249	NE2	HIS	Α	280	-22.028	23.493	64.660	1.00	46.60
1250	CD2	HIS			-23.283	23.969	64.964		45.31
1251	С			280	-26.590	23.569	68.343		37.33
1252	0			280	-27.040	22.566	68.911	1.00	
1253	N	ALA			-27.212	24.737			36.55
1254	CA			281	-28.494	25.000	68.825		38.46
1255	СВ			281	-28.828	26.461	68.875		37.40
1256	С			281	-29.597	24.175	68.213		41.55
1257	0			281	-29.485	23.958	67.009		41.26
1258	N			282	-30.764	24.290	68.822		41.87
1259	CA			282	-31.606	23.344	69.535		41.68
1260	CB			282	-32.618	22.859	68.482		42.55
1261	CG			282	-32.233	23.675	67.281		41.31
1262	CD			282	-31.631	25.026	67.910		44.02
1263	С			282	-30.712	22.264	70.155		40.86
1264	O			282	-30.004	21.537	69.457		40.78
1265	N C7			283	-30.704	22.233	71.483		38.89
1266	CA	SEK	А	283	-30.011	21.158	72.148	1.00	39.04

### FIGURE 3Y

А	В	С	D	E	F	G	Н	I	J
1267	СВ	SER	Α	283	-28.515	21.411	72.222	1.00	38.52
1268	OG	SER	Α	283	-27.832	20.358	72.915	1.00	40.61
1269	С	SER			-30.549	20.857	73.526	1.00	39.37
1270	0	SER	Α	283	-31.163	21.706	74.190	1.00	39.84
1271	N	SER	Α	284	-30.310	19.641	73.955	1.00	39.43
1272	CA	SER	Α	284	-30.584	19.299	75.314	1.00	41.76
1273	CB	SER	Α	284	-31.245	17.940	75.356	1.00	43.22
1274	OG	SER	Α	284	-32.242	17.954	76.372	1.00	47.58
1275	С	SER	Α	284	-29.239	19.218	75.979	1.00	42.43
1276	0	SER	Α	284	-28.205	19.677	75.432	1.00	43.18
1277	N	ARG	Α	285	-29.226	18.626	77.161	1.00	42.91
1278	CA	ARG	Α	285	-27.980	18.390	77.875	1.00	43.85
1279	СВ	ARG	Α	285	-27.914	19.247	79.145	1.00	43.75
1280	CG	ARG	Α	285	-26.582	19.105	79.889	1.00	43.99
1281	CD	ARG	Α	285	-26.415	20.119	81.009	1.00	45.74
1282	NE	ARG	Α	285	-27.612	20.161	81.838	1.00	49.71
1283	CZ	ARG	Α	285	-27.710	19.525	82.988	1.00	52.93
1284	NH1	ARG	Α	285	-28.822	19.597	83.713	1.00	53.76
1285	NH2	ARG	Α	285	-26.675	18.805	83.415	1.00	55.88
1286	С	ARG			-27.906	16.906	78.267	1.00	43.69
1287	0	ARG			-28.836	16.435	78.958	1.00	44.26
1288	N	THR	Α	288	-25.116	15.611	79.501	1.00	47.82
1289	CA			288	-23.866	15.594	80.345	1.00	48.76
1290	СВ			288	-22.675	16.360	79.646	1.00	48.89
1291	OG1	THR			-22.479	15.933	78.293	1.00	51.35
1292	CG2	THR			-21.345	16.015	80.297	1.00	47.79
1293	C	THR			-24.101	16.243	81.732	1.00	49.14
1294	0	THR			-24.852	17.214	81.851	1.00	47.49
1295	N	LEU			-23.443	15.702	82.757	1.00	50.43
1296	CA	LEU			-23.441	16.283	84.118	1.00	53.20
1297	СВ	LEU			-22.802	15.267	85.056	1.00	53.63
1298	CG	LEU			-23.766	14.793	86.121	1.00	57.03
1299	CD1	LEU			-24.112	15.959	87.046	1.00	59.33
1300	CD2	LEU			-25.011	14.189	85.463	1.00	60.93
1301	C	LEU			-22.694	17.651	84.276	1.00	53.31
1302	0	LEU			-21.619	17.817	83.725	1.00	53.60
1303	N	CYS			-23.229	18.557	85.113	1.00	55.50
1304	CA	CYS			-22.752	19.970	85.335		57.08
1305	СВ	CYS			-23.926	20.833	85.843		57.49
1306	SG			290	-25.205	21.169	84.585		64.10
1307	С			290	-21.426	20.313	86.110	1.00	56.52
1308	0	CYS			-20.448	19.597	85.933		
1309	N	GLY			-21.379	21.417	86.898	1.00	55.52
1310	CA	GLY			-20.169	21.921	87.613		52.28
1311	C	GLY			-20.635	23.035	88.583	1.00	50.12
1312	0	GLY			-21.578	22.837	89.335	1.00	
1313	N			292	-20.005	24.208	88.624		47.90
1314	CA			292	-20.610	25.273	89.444		44.87
1315	СВ			292	-19.672	26.461	89.703		47.07
1316	OG1			292	-20.442	27.619	90.103		47.16
1317	CG2	THR			-19.180	26.950	88.383		48.62

## FIGURE 3Z

A	В	С	D	E	F	G	Н	I	J
1318	С	THR	Α	292	-21.798	25.781	88.602	1.00	41.88
1319	0			292	-21.634	25.980	87.395		41.81
1320	N			293	-22.964	26.018	89.200	1.00	36.57
1321	CA			293	-24.101	26.475	88.391	1.00	35.69
1322	СВ			293	-25.398	26.116	89.074	1.00	35.41
1323	CG			293	-26.168	24.807	88.850	1.00	42.89
1324	CD1			293	-25.377	23.623	88.364	1.00	
1325	CD2			293	-27.014	24.434	90.111	1.00	
1326	CDZ			293	-24.158	27.975	88.146	1.00	
1327	0			293	-25.017	28.435	87.395	1.00	32.15
1327	N			294	-23.017	28.729	88.755	1.00	31.34
1329				294	-23.240	30.191	88.780	1.00	
1329	CA CB			294		30.788		1.00	30.17
1331	CG				-22.072	30.766	89.362	1.00	31.41
1331		ASP		294	-22.096 -21.149	30.773	90.875 91.449	1.00	36.52
1333		ASP		294	-23.074 -23.740	31.224	91.535	1.00	
1334	C			294	-23.740	30.941	87.510	1.00	
1335 1336	O			294		31.966	87.568		28.82
	N				-23.192 -23.409	30.486	86.390		28.35
1337	CA			295		31.144	85.110		29.18
1338 1339	CB			295 295	-22.081 -21.064	31.134	84.392	1.00	
1340	CG CD1			295	-21.064	31.857	85.196	1.00	
1341	CE1			295	-20.229 -19.281	31.183 31.854	86.080 86.858	1.00	
1341	CZ			295	-19.251 -19.257	33.216	86.782	1.00	
1342	OH			295	-18.331	33.880	87.548	1.00	39.27
1344	CE2	TYR			-20.078	33.903	85.910	1.00	33.69
1345	CD2			295	-20.983	33.215	85.124	1.00	32.42
1346	C			295	-24.468	30.562	84.180	1.00	30.12
1347	0			295	-24.606	31.005	83.032	1.00	29.57
1348	N			296	-25.192	29.556	84.637	1.00	
1349	CA			296	-26.160	28.872	83.753	1.00	30.57
1350	СВ			296	-26.090	27.394	83.996	1.00	
1351	CG			296	-24.686	26.827	83.787		36.71
1352	CD1			296	-24.675	25.310	84.148	1.00	38.55
1353	CD2	LEU			-24.209	27.111	82.373	1.00	35.88
1354	C			296	-27.547	29.301	84.042	1.00	30.06
1355	0			296	-27.902	29.441			28.76
1356	N			297	-28.346	29.432	82.969		29.59
1357	CA			297	-29.752	29.814	83.035		29.63
1358	СВ			297	-30.105	30.142	81.563		30.10
1359	CG			297	-29.256	29.232	80.816		30.36
1360	CD			297	-27.902	29.176	81.578		30.37
1361	C			297	-30.593	28.606	83.518		30.53
1362	0			297	-30.133	27.475	83.493		29.72
1363	N	PRO	Α	298	-31.785	28.907	83.980		32.38
1364	CA	PRO	Α	298	-32.748	27.911	84.486		35.25
1365	СВ	PRO	Α	298	-34.030	28.716	84.623		34.69
1366	CG	PRO	Α	298	-33.555	30.121	84.897	1.00	35.48
1367	CD	PRO	Α	298	-32.269	30.280	84.096		32.59
1368	С	PRO	Α	298	-32.951	26.766	83.492	1.00	37.27

### FIGURE 3AA

A	В	С	D	E	F	G	Н	I	J
1369	0	PR∩	Δ	298	-32.829	25.611	83.920	1.00	38.20
1370	N			299	-33.089	27.056	82.197	1.00	38.20
1371	CA	GLU			-33.396	25.984	81.252	1.00	
1371	CB	GLU			-33.745	26.499	79.833	1.00	39.94
	CG								
1373		GLU			-32.614	27.242	79.139	1.00	39.16
1374	CD OF1	GLU			-32.578	28.754	79.410	1.00	39.82
1375	OE1			299	-33.124	29.242	80.436	1.00	37.57
1376	OE2			299	-31.980	29.467	78.564	1.00	37.07
1377	С			299	-32.299	24.969	81.174		41.23
1378	0	GLU			-32.543	23.747	81.097		41.06
1379	N	MET		300	-31.075	25.468	81.248		41.85
1380	CA	MET		300	-29.951	24.596	81.206		43.22
1381	СВ	MET		300	-28.679	25.376	81.027	1.00	43.88
1382	CG	MET		300	-27.499	24.515	81.020	1.00	
1383	SD	MET		300	-26.839	24.501	79.396	1.00	
1384	CE	MET		300	-25.544	23.343	79.572	1.00	54.71
1385	С	MET		300	-29.837	23.750	82.461	1.00	44.15
1386	0	MET		300	-29.682	22.512	82.356		44.33
1387	N	ILE		301	-29.864	24.362	83.638		44.85
1388	CA			301	-29.735	23.521	84.831		46.79
1389	СВ	ILE		301	-29.657	24.332	86.111	1.00	
1390	CG1			301	-30.818	25.308	86.276	1.00	50.37
1391	CD1			301	-30.163	26.709	86.641	1.00	56.06
1392	CG2			301	-28.369	25.222	86.119	1.00	
1393	С	ILE		301	-30.836	22.441	84.891	1.00	48.14
1394	0	ILE		301	-30.538	21.258	85.093		48.00
1395	N	GLU			-32.085	22.854	84.677		49.20
1396	CA	GLU			-33.236	21.952	84.671		51.02
1397	СВ	GLU			-34.520	22.754	84.559	1.00	51.41
1398	CG	GLU			-34.831	23.576	85.792	1.00	55.27
1399	CD	GLU			-35.798	24.695	85.474	1.00	59.81
1400	OE1	GLU			-36.087	25.555	86.349	1.00	63.64
1401	OE2	GLU			-36.294	24.693	84.335	1.00	60.77
1402	С	GLU			-33.242	20.937	83.540	1.00	51.10
1403	0	GLU			-34.179	20.143	83.434	1.00	51.91
1404	N	GLY GLY			-32.240	20.988	82.669	1.00	50.72
1405	CA				-32.155	20.071	81.553		49.63
	С	GLY			-33.262				49.30
1407	O	GLY			-33.624	19.227	79.864		50.60
1408	N	ARG			-33.809	21.402	80.323		47.24
1409	CA	ARG			-34.799	21.609	79.256		46.04
1410	CB	ARG			-35.716	22.800	79.591		46.73
1411	CG	ARG			-36.712	22.504	80.773		49.63
1412	CD	ARG			-37.419	23.759	81.406		55.75
1413	NE	ARG			-37.497	24.898	80.477	1.00	58.41
1414	CZ NH1	ARG			-37.277	26.172	80.822		60.70
1415	NH1	ARG			-37.360 -36.965	27.151	79.903		61.20
1416	NH2	ARG			-36.965	26.473	82.083 77.907		58.65 44.67
1417	С	ARG			-34.097	21.838 21.996	77.852		
1418	O N			304	-32.861				43.50
1419	Ν	ME T	А	305	-34.858	21.822	76.819	T.00	41.82

### FIGURE 3AB

A	В	С	D	E	F	G	Н	I	J
1420	CA	MET	7\	305	-34.254	22.089	75.503	1 00	42.19
1421	CB			305	-35.229	21.851	74.333		41.21
1421	CG	MET		305	-35.426	20.357	73.940	1.00	
1423	SD	MET		305	-33.420	19.263	73.940	1.00	
1423								1.00	
	CE			305	-33.530	19.109	72.178		55.74
1425	С			305	-33.865	23.563	75.506	1.00	38.86
1426	0	MET		305	-34.562	24.353	76.091	1.00	38.98
1427	N			306	-32.786	23.933	74.838	1.00	37.11
1428	CA			306	-32.358	25.332	74.903	1.00	36.23
1429	СВ			306	-31.486	25.515	76.164	1.00	34.70
1430	CG			306	-30.350	24.541	76.239	1.00	31.57
1431		HIS			-30.436	23.353	76.920	1.00	30.19
1432		HIS			-29.306	22.688	76.809	1.00	31.98
1433		HIS			-28.485	23.405	76.061	1.00	
1434	CD2	HIS			-29.117	24.569	75.698	1.00	31.19
1435	С			306	-31.570	25.711	73.662	1.00	36.80
1436	0			306	-31.106	24.834	72.897	1.00	36.60
1437	Ν	ASP			-31.378	27.017	73.498	1.00	37.06
1438	CA	ASP			-30.728	27.538	72.310	1.00	37.90
1439	СВ	ASP			-31.778	27.990	71.294	1.00	38.38
1440	CG	ASP	Α	307	-32.671	29.159	71.810	1.00	43.93
1441	OD1	ASP	Α	307	-33.590	29.626	71.077	1.00	51.28
1442	OD2	ASP	Α	307	-32.554	29.695	72.926	1.00	43.92
1443	С	ASP	Α	307	-29.824	28.702	72.622	1.00	37.59
1444	0	ASP	Α	307	-29.361	28.848	73.739	1.00	37.38
1445	N	GLU	Α	308	-29.676	29.585	71.642	1.00	36.80
1446	CA	GLU	Α	308	-28.726	30.683	71.742	1.00	37.37
1447	CB	GLU	Α	308	-28.825	31.551	70.492	1.00	37.85
1448	CG	GLU	Α	308	-28.228	30.905	69.266	1.00	40.29
1449	CD	GLU	Α	308	-29.197	29.990	68.528	1.00	45.91
1450	OE1	GLU	Α	308	-30.253	29.629	69.089	1.00	43.52
1451	OE2	GLU	Α	308	-28.879	29.616	67.361	1.00	48.59
1452	С	GLU	Α	308	-29.008	31.574	72.946	1.00	35.64
1453	0	GLU	Α	308	-28.099	32.237	73.434	1.00	34.56
1454	N	LYS	Α	309	-30.247	31.603	73.410	1.00	33.77
1455	CA	LYS	Α	309	-30.557	32.491	74.535	1.00	33.68
1456	СВ	LYS	Α	309	-32.071	32.589	74.813	1.00	34.13
1457	CG	LYS	Α	309	-32.853	33.190	73.626	1.00	35.58
1458	CD	LYS	Α	309	-32.289	34.571	73.302	1.00	39.16
1459	CE	LYS	Α	309	-33.289	35.387	72.485	1.00	46.27
1460	NΖ	LYS	Α	309	-34.624	35.259	73.121	1.00	46.60
1461	С	LYS	Α	309	-29.793	32.123	75.816	1.00	32.90
1462	0	LYS	Α	309	-29.673	32.945	76.708	1.00	32.40
1463	N	VAL			-29.242	30.932	75.870		31.17
1464	CA	VAL			-28.473	30.508	77.022		32.76
1465	СВ			310	-27.993	29.086	76.822	1.00	
1466	CG1	VAL			-26.762	28.825	77.639		36.49
1467	CG2	VAL			-29.154	28.095	77.249		32.68
1468	С			310	-27.292	31.457	77.250		33.09
1469	0			310	-27.083	31.951	78.365		31.77
1470	N	ASP	Α	311	-26.568	31.770	76.175	1.00	31.32

## FIGURE 3AC

A	В	С	D	E	F	G	Н	I	J
1471	CA	ASP	Δ	311	-25.422	32.682	76.275	1 00	32.19
1472	CB	ASP			-24.578	32.656	74.950		32.21
1473	CG	ASP			-23.893	31.256	74.696	1.00	
1474		ASP			-23.601	30.482	75.635	1.00	
		ASP			-23.601	30.402			
1475							73.584		34.64
1476	С	ASP			-25.848	34.089	76.674		31.34
1477	0	ASP			-25.054	34.819	77.265		31.50
1478	N			312	-27.074	34.500	76.349		30.65
1479	CA			312	-27.540	35.829	76.741		30.65
1480	СВ			312	-28.880	36.194	76.114	1.00	
1481	CG			312	-28.740	36.747	74.676		33.15
1482	CD1	LEU			-27.998	38.080	74.782		37.24
1483	CD2	LEU			-27.978	35.740	73.770		37.98
1484	С			312	-27.659	35.915	78.252		30.10
1485	0	LEU	Α	312	-27.212	36.882	78.870		29.74
1486	N			313	-28.221	34.878	78.847		28.70
1487	CA			313	-28.290	34.885	80.311	1.00	29.18
1488	CB	TRP	Α	313	-28.980	33.655	80.774	1.00	29.28
1489	CG	TRP	Α	313	-28.856	33.398	82.197	1.00	29.13
1490	CD1	TRP	Α	313	-27.798	32.871	82.848	1.00	26.72
1491	NE1	TRP	Α	313	-28.104	32.728	84.184	1.00	28.25
1492	CE2	TRP	Α	313	-29.402	33.129	84.370	1.00	28.86
1493	CD2	TRP	Α	313	-29.877	33.584	83.145	1.00	26.93
1494	CE3	TRP	Α	313	-31.192	34.028	83.062		26.93
1495	CZ3			313	-31.969	34.038	84.199	1.00	31.77
1496	CH2			313	-31.450	33.635	85.422		28.09
1497	CZ2			313	-30.175	33.170	85.538		26.06
1498	С			313	-26.880	34.959	80.918		29.84
1499	0			313	-26.633	35.738	81.823		27.08
1500	N			314	-25.958	34.152	80.409		29.72
1501	CA			314	-24.593	34.162	80.901		30.37
1502	СВ			314	-23.777	33.087	80.139		30.46
1503	OG			314	-24.244	31.776	80.494		35.30
1504	C			314	-23.937	35.568	80.801		31.13
1505	0			314	-23.199	35.980	81.679		27.77
1506	N			315	-24.183	36.276	79.708		30.52
1507	CA	LEU			-23.699	37.630	79.537	1.00	
1508		LEU			-24.303	38.182	78.258		31.92
1509	CG			315	-23.556	39.322	77.630		34.89
1510	CD1	LEU			-22.077	38.966	77.617		32.65
1511	CD1	LEU			-24.094	39.490	76.207		34.24
1512	C D Z			315	-24.189	38.521	80.657		30.26
1513	0			315	-23.467	39.375	81.154		29.93
					-25.416		81.084		31.24
1514	N C7	GLY		316	-25.410 -26.030	38.270 39.018	82.160		
1515	CA								28.40
1516	С			316	-25.336	38.709	83.470		29.31
1517	O N	GLY			-24.989	39.635	84.232		28.62
1518	N	VAL			-25.123	37.426	83.751		29.39
1519	CA	VAL			-24.392	37.045	84.964		29.86
1520	CB			317	-24.272				29.69
1521	CGI	VAL	А	31/	-23.433	35.135	86.302	1.00	31.40

### FIGURE 3AD

A	В	С	D	E	F	G	Н	I	J
1522	CG2	VAL	7\	217	-25.625	34.885	85.201	1.00	30.52
1523	CGZ	VAL			-23.023	37.715	84.961		30.09
1524	0	VAL			-22.525	38.275	85.976		28.93
1525	N			318	-22.323	37.665	83.832	1.00	29.07
1526									
	CA	LEU			-20.973	38.219	83.759	1.00	
1527	CB			318	-20.327	37.940	82.391	1.00	29.62 33.45
1528	CG	LEU			-19.795	36.566	82.116		
1529	CD1	LEU			-19.343	36.587	80.606	1.00	31.59
1530	CD2	LEU			-18.570	36.186	83.001		26.99
1531	С			318	-21.015	39.716	83.938		29.78
1532	0			318	-20.140	40.243	84.572		29.27
1533	N	CYS			-22.036	40.401	83.423		29.91
1534	CA	CYS			-22.072	41.831	83.606	1.00	31.51
1535	CB	CYS			-23.214	42.431	82.818	1.00	31.68
1536	SG	CYS			-23.007	44.241	82.719	1.00	
1537	С			319	-22.152	42.216	85.116	1.00	31.22
1538	0	CYS			-21.439	43.092	85.632		29.46
1539	N			320	-22.985	41.482	85.819		29.74
1540	CA			320	-23.149	41.689	87.243	1.00	
1541	CB			320	-24.320	40.843	87.746		28.54
1542	CG			320	-24.606	40.973	89.212		28.67
1543	CD1			320	-23.746	40.436	90.152	1.00	28.63
1544	CE1 CZ			320 320	-24.037	40.574	91.521 91.901	1.00	31.25
1545 1546	OH			320	-25.218 -25.601	41.261	93.204	1.00	27.73 34.97
1547	CE2			320		41.384	91.016		
1548	CD2			320	-26.070 -25.745	41.711 41.625	89.636		28.41 27.53
1549	CDZ			320	-21.810	41.373	87.977	1.00	
1550	0			320	-21.286	42.208	88.741		28.99
1551	N	GLU			-21.252	40.185	87.727		28.26
1552	CA	GLU			-19.996	39.790	88.381	1.00	29.29
1553	CB	GLU			-19.511	38.398	87.976		27.46
1554	CG	GLU			-18.367	37.989	88.874		31.39
1555	CD	GLU			-17.939	36.565	88.757		39.04
1556	OE1	GLU			-16.893	36.204	89.386	1.00	40.16
1557	OE2	GLU			-18.629	35.792	88.062	1.00	41.43
1558	C	GLU			-18.858	40.810	88.173		29.09
1559	0	GLU			-18.148		89.112		28.70
1560	N			322	-18.712	41.290	86.942		28.18
1561	CA			322	-17.690	42.282	86.620		29.59
1562	СВ			322	-17.742	42.671	85.130		30.02
1563	CG			322	-17.277	41.578	84.189		29.13
1564	CD1			322	-16.706	40.416	84.659		29.70
1565	CE1	PHE			-16.287	39.422	83.772		32.17
1566	CZ			322	-16.416	39.619	82.418		33.54
1567	CE2			322	-16.981	40.753	81.954		33.04
1568	CD2	PHE			-17.412	41.738	82.844		30.45
1569	С	PHE	Α	322	-17.874	43.526	87.468	1.00	30.51
1570	0	PHE	Α	322	-16.924	44.017	88.092	1.00	32.18
1571	N	LEU	Α	323	-19.079	44.047	87.443	1.00	30.76
1572	CA	LEU	Α	323	-19.461	45.235	88.188	1.00	31.93

## FIGURE 3AE

1573 CB LEU A 323	A
1574 CG LEU A 323	1572
1575 CD1 LEU A 323	
1576 CD2 LEU A 323	
1577 C LEU A 323	
1578 O LEU A 323	
1579 N VAL A 324 -19.868 43.827 90.139 1.00 33.6 1580 CA VAL A 324 -20.061 43.630 91.587 1.00 33.2 1581 CB VAL A 324 -21.449 42.976 91.860 1.00 33.8 1582 CG1 VAL A 324 -21.709 42.622 93.380 1.00 32.6 1583 CG2 VAL A 324 -22.586 43.857 91.300 1.00 34.2 1584 C VAL A 324 -18.928 42.911 92.263 1.00 35.5 1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.642 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1580 CA VAL A 324 -20.061 43.630 91.587 1.00 33.2 1581 CB VAL A 324 -21.449 42.976 91.860 1.00 33.8 1582 CG1 VAL A 324 -21.709 42.622 93.380 1.00 32.6 1583 CG2 VAL A 324 -22.586 43.857 91.300 1.00 34.2 1584 C VAL A 324 -18.928 42.911 92.263 1.00 35.5 1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1581 CB VAL A 324	
1582 CG1 VAL A 324 -21.709 42.622 93.380 1.00 32.6 1583 CG2 VAL A 324 -22.586 43.857 91.300 1.00 34.2 1584 C VAL A 324 -18.928 42.911 92.263 1.00 35.5 1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1583 CG2 VAL A 324 -22.586 43.857 91.300 1.00 34.2 1584 C VAL A 324 -18.928 42.911 92.263 1.00 35.5 1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1584 C VAL A 324 -18.928 42.911 92.263 1.00 35.5 1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1585 O VAL A 324 -18.642 43.145 93.424 1.00 35.3 1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1586 N GLY A 325 -18.226 42.038 91.560 1.00 35.5 1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1587 CA GLY A 325 -17.194 41.273 92.225 1.00 35.3 1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1588 C GLY A 325 -17.594 39.835 92.535 1.00 36.0 1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1589 O GLY A 325 -16.746 39.003 92.813 1.00 37.0 1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1590 N LYS A 326 -18.880 39.528 92.442 1.00 35.2	
1591 CA LYS A 326 -19.304 38.161 92.638 1.00 35.8	
1592 CB LYS A 326 -19.650 37.922 94.122 1.00 35.9	
1593 CG LYS A 326 -20.941 38.598 94.489 1.00 40.0	
1594 CD LYS A 326 -21.233 38.587 96.024 1.00 47.4	
1595 CE LYS A 326 -22.214 39.748 96.321 1.00 51.8	
1596 NZ LYS A 326 -21.819 40.553 97.484 1.00 48.8	
1597 C LYS A 326 -20.512 37.929 91.754 1.00 33.8	
1598 O LYS A 326 -21.227 38.853 91.451 1.00 31.5	
1599 N PRO A 327 -20.755 36.691 91.332 1.00 33.5 1600 CA PRO A 327 -21.927 36.437 90.463 1.00 32.7	
1601 CB PRO A 327 -21.678 34.994 89.969 1.00 33.9	
1602 CG PRO A 327 -21.076 34.347 91.241 1.00 35.3	
1603 CD PRO A 327 -19.983 35.449 91.621 1.00 33.3	
1604 C PRO A 327 -23.245 36.595 91.255 1.00 30.8	
1605 O PRO A 327 -23.300 36.380 92.463 1.00 32.1	
1606 N PRO A 328 -24.309 36.989 90.598 1.00 29.6	
1607 CA PRO A 328 -25.541 37.336 91.315 1.00 29.9	
1608 CB PRO A 328 -26.396 37.936 90.249 1.00 28.2	
1609 CG PRO A 328 -25.879 37.253 88.972 1.00 30.6	
1610 CD PRO A 328 -24.406 37.239 89.158 1.00 29.0	
1611 C PRO A 328 -26.291 36.189 92.066 1.00 32.0	
1612 O PRO A 328 -27.110 36.498 92.935 1.00 31.5	
1613 N PHE A 329 -26.007 34.919 91.745 1.00 30.7	
1614 CA PHE A 329 -26.723 33.835 92.391 1.00 32.1	
1615 CB PHE A 329 -27.367 32.923 91.329 1.00 30.3	
1616 CG PHE A 329 -28.198 33.663 90.371 1.00 29.1	
1617 CD1 PHE A 329 -29.349 34.294 90.783 1.00 26.8	
1618 CE1 PHE A 329 -30.109 35.003 89.921 1.00 26.7	
1619 CZ PHE A 329 -29.692 35.115 88.583 1.00 29.1	
1620 CE2 PHE A 329 -28.507 34.503 88.156 1.00 28.2	
1621 CD2 PHE A 329 -27.779 33.782 89.042 1.00 29.1	
1622 C PHE A 329 -25.833 33.027 93.287 1.00 33.3	1622
1623 O PHE A 329 -26.260 31.988 93.763 1.00 35.5	1623

### FIGURE 3AF

A	В	С	D	E	F	G	Н	I	J
1624	NT	CTII	7\	330	-24.623	33.505	93.513	1 00	35.42
1625	N CA			330	-24.623	32.877	94.397	1.00	
1626	CB			330	-23.636	33.906	94.397	1.00	39.72
							94.700		
1627	CG			330	-21.251	33.325			44.21
1628	CD			330	-20.378	34.364	95.894	1.00	53.19
1629	OE1	GLU		330	-20.779	34.883	96.993	1.00	53.55
1630	OE2	GLU			-19.295	34.665	95.337	1.00	58.16
1631	С	GLU			-24.373	32.498	95.704	1.00	39.04
1632	0			330	-25.175	33.269	96.217	1.00	37.84
1633	N	ALA			-24.084	31.303	96.200	1.00	
1634	CA			331	-24.680	30.771	97.425	1.00	40.27
1635	СВ			331	-26.002	30.149	97.126	1.00	
1636	С	ALA			-23.658	29.753	97.888	1.00	
1637	0	ALA			-22.757	29.404	97.127	1.00	
1638	N	ASN			-23.776	29.280	99.121		41.89
1639	CA			332	-22.737	28.404	99.662		40.88
1640	СВ			332	-22.602		101.220		43.11
1641	CG			332	-21.784	29.826	101.626		48.66
1642	OD1	ASN			-20.570	29.937	101.359	1.00	
1643	ND2	ASN			-22.462	30.786	102.245	1.00	55.15
1644	С			332	-23.050	26.959	99.235	1.00	37.57
1645	0			332	-22.225	26.050	99.332		39.59
1646	N			333	-24.231	26.755	98.724		36.44
1647	CA			333	-24.536	25.410	98.298	1.00	
1648	СВ			333	-25.645	24.665	99.264		37.09
1649	OG1			333	-25.097		100.596		40.58
1650	CG2			333	-25.650	23.188	99.046		42.78
1651	С			333	-24.981	25.425	96.865		34.33
1652	0			333	-25.642	26.372	96.398		33.08
1653	N			334	-24.713	24.319	96.190		34.09
1654	CA			334	-25.181	24.137	94.830		33.28
1655	СВ			334	-24.748	22.746	94.425	1.00	34.15
1656	CG			334	-25.241	22.198	93.148	1.00	
1657	CD1			334	-24.367	22.102	92.069		
1658	CE1			334	-24.765	21.536	90.885		41.47
1659	CZ			334	-26.025	21.028	90.764		45.44
1660	OH			334	-26.316	20.439	89.536	1.00	53.44
1661	CE2			334	-26.931	21.076			41.49
1662		TYR			-26.535	21.644	93.021		39.26
1663	С			334	-26.682	24.162	94.837		34.00
1664	0			334	-27.330	24.686	93.921		32.29
1665	N	GLN			-27.263	23.490	95.830	1.00	33.92
1666	CA	GLN			-28.698	23.382	95.856		
1667	СВ	GLN			-29.136	22.355	96.934		36.44
1668	CG			335	-28.819	20.855	96.503		37.94
1669	CD			335	-27.495	20.276	97.085		40.55
1670	OE1	GLN			-27.461	19.102	97.552		37.86
1671	NE2	GLN			-26.437	21.088	97.108		36.60
1672	С			335	-29.324	24.794	96.037		34.20
1673	0			335	-30.282	25.140	95.379		35.30
1674	N	GЪŪ	А	336	-28.791	25.559	96.942	1.00	32.77

## FIGURE 3AG

А	В	С	D	Ε	F	G	Н	I	J
1675	CA	GLU	Α	336	-29.205	26.915	97.201	1.00	34.44
1676	СВ			336	-28.385	27.265	98.440	1.00	
1677	CG			336	-28.352	28.650	99.013	1.00	
1678	CD			336	-27.092	28.866	99.875	1.00	50.58
1679	OE1	GLU			-25.978	28.319	99.620	1.00	58.53
1680	OE2	GLU			-27.126	29.678	100.790	1.00	40.31
1681	C			336	-28.995	27.811	95.873	1.00	33.80
1682	0			336	-29.877	28.563	95.449	1.00	31.17
1683	И			337	-27.868	27.635	95.191	1.00	32.08
1684	CA	THR			-27.662	28.368	93.945	1.00	31.48
1685	CB	THR			-26.235	28.047	93.405	1.00	30.08
1686	OG1	THR			-25.313	28.487	94.390	1.00	33.00
1687	CG2	THR			-25.906	28.929	92.159	1.00	
1688	CGZ			337	-28.724	28.055	92.139	1.00	
1689	0			337	-29.235	28.932	92.247		28.46
1690									
	N			338	-29.027	26.756 26.309	92.754	1.00	30.17
1691 1692	CA			338	-30.049		91.844	1.00	31.26
	CB			338	-30.212 -31.212	24.805	92.063	1.00	33.22
1693	CG			338		24.185	91.144	1.00	39.22
1694	CD1 CE1	TYR			-30.800	23.567	89.964	1.00	
1695		TYR			-31.709	22.969	89.124	1.00	
1696 1697	CZ OH			338	-33.058	23.003 22.431	89.460	1.00	51.06
1698	CE2			338 338	-33.992 -33.479	23.615	88.628 90.622	1.00	55.33 46.29
1699	CD2	TYR			-32.560	24.179	91.462	1.00	
1700	CD2			338	-31.396	27.002	92.147	1.00	30.29
1701	0			338	-32.102	27.472	91.277	1.00	
1702	N	ALA			-31.739	27.026	93.411		29.94
1703	CA	ALA			-32.984	27.737	93.804	1.00	
1704	CB	ALA			-33.149	27.684	95.338	1.00	30.49
1705	C	ALA			-32.960	29.196	93.377	1.00	
1706	0	ALA			-33.915	29.676	92.798	1.00	30.50
1707	N			340	-31.867	29.875	93.686	1.00	
1708	CA			340	-31.708	31.285	93.348		29.69
1709	СВ	ARG			-30.375	31.804	93.896		29.56
1710	CG	ARG			-30.447	31.776	95.494	1.00	
1711	CD	ARG			-31.154	32.954	96.011	1.00	39.53
	NE	ARG	Α	340	-30.493				45.06
1713	CZ	ARG			-29.323				45.59
1714		ARG			-28.683				44.01
1715		ARG			-28.835				44.77
1716	С	ARG	Α	340	-31.871	31.547		1.00	29.56
1717	0			340	-32.649	32.431	91.413		29.84
1718	N	ILE	Α	341	-31.248	30.679	91.087	1.00	29.70
1719	CA	ILE	Α	341	-31.279	30.831	89.641	1.00	27.75
1720	СВ	ILE	Α	341	-30.265	29.851	89.077	1.00	27.48
1721	CG1	ILE	Α	341	-28.835	30.335	89.281	1.00	24.64
1722	CD1	ILE	А	341	-27.801	29.268	88.849		27.34
1723	CG2	ILE	А	341	-30.531	29.617	87.612	1.00	28.09
1724	С			341	-32.653				28.03
1725	0	ILE	Α	341	-33.236	31.391	88.388	1.00	29.33

## FIGURE 3AH

A	В	С	D	Ε	F	G	j	Н	I	J
1726	N	SER	7\	3/12	-33.25	8 29.4	70 00	.585	1 00	30.95
1727	CA			342	-34.58			.125		31.90
1728	CB	SER			-34.97			822	1.00	33.11
1729	OG	SER							1.00	
		SER			-36.33			0.665		42.55
1730	С				-35.59			.400	1.00	32.49
1731	0	SER			-36.44			3.565	1.00	35.12
1732	N	ARG			-35.47			).559	1.00	31.84
1733	CA	ARG			-36.38			).917	1.00	32.56
1734	CB	ARG			-36.53			2.470	1.00	33.12
1735	CG	ARG			-37.17			3.099	1.00	36.80
1736	CD	ARG			-36.95			1.628		43.39
1737	NE	ARG			-37.67			344	1.00	
1738	CZ	ARG			-38.08			1.847	1.00	55.23
1739		ARG			-37.86			3.587	1.00	58.10
1740	NH2	ARG			-38.71			6.654	1.00	55.82
1741	С	ARG			-35.91			386	1.00	32.02
1742	0	ARG			-36.64			.481	1.00	31.13
1743	N	VAL			-34.71			766	1.00	32.93
1744	CA	VAL			-34.04			312	1.00	33.02
1745	CB	VAL			-34.60			3.032	1.00	33.79
1746	CG1	LAV			-33.54			7.403	1.00	33.57
1747	CG2	LAV			-35.02			7.041	1.00	34.92
1748 1749	С	VAL VAL			-33.99			).479	1.00	31.91
	0				-34.39			.393	1.00	32.52
1750 1751	N CA	GLU GLU			-33.50 -33.50			.597	1.00	33.06 35.54
1752	CB	GLU			-34.04			3.988	1.00	37.02
1753	CG	GLU			-33.65			1.122	1.00	
1754	CD	GLU			-34.18			5.428	1.00	
1755	OE1	GLU			-34.61			5.347	1.00	58.06
1756	OE2	GLU			-34.13			5.554	1.00	58.84
1757	C	GLU			-32.13			2.961	1.00	33.87
1758	0	GLU			-31.18			3.332	1.00	33.72
1759	N	PHE			-32.04			2.694	1.00	32.77
1760	CA	PHE			-30.81			2.902	1.00	32.91
1761	СВ	PHE			-29.90			.657	1.00	33.13
1762	CG	PHE			-30.43			.469	1.00	34.17
1763		PHE			-31.33			647		36.56
1764		PHE			-31.83			3.527		35.71
1765	CZ			346	-31.46			3.220		38.88
1766		PHE			-30.56			0.037		38.32
1767		PHE			-30.01			.146		39.09
1768	С			346	-31.13			3.174		33.06
1769	0			346	-32.20			2.785		32.92
1770	N			347	-30.22			3.853		32.73
1771	CA	THR			-30.38			1.108		33.76
1772	СВ	THR			-30.75			5.597		33.91
1773	OG1	THR	Α	347	-29.77	6 41.8	370 96	5.415		35.21
1774	CG2	THR	Α	347	-32.06	7 41.7	98 96	5.015	1.00	33.87
1775	С	THR	Α	347	-29.02			3.850		33.74
1776	Ο	THR	Α	347	-27.99	8 42.1	.42 93	3.915	1.00	34.60

## FIGURE 3AI

A	В	С	D	E	F	G	Н	I	J
1777	N	DUE	7\	348	-29.028	44.146	93.635	1.00	33.51
1778	N CA			348	-27.835	44.140	93.033	1.00	33.28
1779	CB	PHE		348	-28.204	45.979	92.254	1.00	32.67
								1.00	
1780	CG CD1			348	-28.626	45.454	90.940		31.24
1781				348	-29.962	45.538	90.551	1.00	32.35
1782	CE1	PHE		348	-30.374	45.068	89.325	1.00	31.74
1783 1784	CZ CE2	PHE PHE		348 348	-29.433	44.491 44.411	88.447	1.00	30.42
1785	CD2	PHE			-28.090 -27.695	44.411	88.822 90.070	1.00	32.15 30.97
1786	CD2			348	-27.093	45.701	94.453	1.00	35.77
1787	0			348	-28.126	46.255	95.209	1.00	35.76
1788	N			349	-26.025	45.772	94.628	1.00	36.99
1789	CA	PRO			-25.493	46.699	95.626	1.00	37.46
1790	CB			349	-23.963	46.485	95.567		38.56
1791	CG			349	-23.670	45.526	94.471	1.00	
1792	CD			349	-24.990	45.029	93.906	1.00	37.24
1793	C			349	-25.883	48.098	95.159	1.00	37.57
1794	0			349	-26.153	48.337	93.990	1.00	36.04
1795	N	ASP			-25.921	49.055	96.076	1.00	39.36
1796	CA			350	-26.257	50.422	95.693		40.98
1797	СВ	ASP			-26.206	51.348	96.903	1.00	42.59
1798	CG	ASP			-27.260	51.031	97.914	1.00	47.11
1799	OD1	ASP			-27.128	51.620	99.016	1.00	53.92
1800	OD2	ASP	Α	350	-28.222	50.225	97.689	1.00	50.42
1801	С	ASP	Α	350	-25.351	51.058	94.663	1.00	40.13
1802	0	ASP	Α	350	-25.814	51.905	93.909	1.00	40.28
1803	N	PHE	Α	351	-24.063	50.736	94.649	1.00	39.85
1804	CA	PHE	Α	351	-23.202	51.402	93.673	1.00	39.47
1805	СВ	PHE	Α	351	-21.718	51.213	93.957	1.00	40.21
1806	CG	PHE	Α	351	-21.278	49.784	93.967	1.00	41.11
1807	CD1	PHE		351	-21.221	49.082	95.162	1.00	39.89
1808	CE1			351	-20.833	47.761	95.192	1.00	
1809	CZ	PHE		351	-20.521	47.111	93.978	1.00	
1810	CE2	PHE		351	-20.589	47.826	92.772	1.00	39.35
1811	CD2	PHE		351	-20.977	49.124	92.767	1.00	41.22
1812	С	PHE		351	-23.543	51.116	92.213	1.00	40.90
1813	0	PHE			-23.177	51.889	91.325		41.02
1814	N	VAL			-24.278	50.042			39.58
1815	CA	VAL			-24.604	49.759	90.531		38.85
1816	CB			352	-25.223	48.351	90.345		37.90
1817	CG1	VAL			-25.491	48.084	88.893		36.19
1818	CG2	VAL			-24.271	47.308	90.902		38.04
1819	С	VAL			-25.531	50.764	89.905		39.39
1820	O N	VAL			-26.631 -25.136	50.985	90.420		38.87 40.16
1821	N			353 353		51.309 52.332	88.742 88.057		40.16
1822 1823	CA CB			353	-25.943 -25.127	53.080	86.987		40.36
1824	OG1			353	-24.703	52.160	85.970		39.47
1825	CG2			353	-23.893	53.625	87.588		39.13
1826	C			353	-27.216	51.852			41.64
1827	0			353	-27.424	50.664	87.152		41.19
,	-			300		55.551	J. • ± U =		

### FIGURE 3AJ

A	В	С	D	E		F		G	F	I	I	J
4000			_			0.54						
1828	N	GLU				.071		816		102		41.67
1829	CA			354		.321		514		485	1.00	
1830	СВ			354		.191		770		372	1.00	46.05
1831	CG			354		.592		252		751		54.41
1832	CD	GLU				.894		090		684	1.00	
1833	OE1	GLU				.014		505		550	1.00	68.68
1834	OE2	GLU				.038		775		551	1.00	67.34
1835	С	GLU				.168		828		156	1.00	
1836	0	GLU				.908		900		858	1.00	
1837	N ~-	GLY				.226		291		353	1.00	
1838	CA	GLY				.041		714		044	1.00	37.79
1839	С	GLY				.598		271		170	1.00	36.84
1840	0			355		.060		403		423	1.00	37.14
1841	Ν			356		.684		016		.092	1.00	36.29
1842	CA			356		.178		669		268	1.00	36.41
1843	СВ			356		.998		660		206	1.00	35.64
1844	С			356		.295		794		782	1.00	35.70
1845	0			356		.490		695		309	1.00	34.90
1846	Ν	ARG				.072		293		745	1.00	36.25
1847	CA			357		.186		504		264	1.00	36.61
1848	СВ			357		.960		250		.339	1.00	36.86
1849	CG	ARG				.169		482		.582	1.00	34.77
1850	CD			357		.988		289		609	1.00	37.61
1851	NE	ARG				.112		640		708	1.00	36.40
1852	CZ			357		.400		468		975	1.00	35.35
1853		ARG				.572		952		320	1.00	39.15
1854		ARG				.498		787		890	1.00	33.56
1855	С	ARG				.165		167		172	1.00	37.12
1856	0			357		.718		074		153	1.00	37.21
1857	Ν	ASP				.420		132		.297	1.00	37.24
1858	CA			358		.353		925		226	1.00	37.93
1859	СВ			358		.614		202		454	1.00	38.87
1860	CG			358		.621		984		324	1.00	
1861		ASP				.846		000		602	1.00	
1862		ASP				.290		788		126		45.46
1863	С	ASP				.868		836		281	1.00	36.98
1864	0	ASP				.656		967		884	1.00	36.97
1865	N	LEU				.578		860		942		35.72
1866	CA			359		.042		867		031		35.51
1867	СВ			359		.595		168		713		35.38
1868	CG			359		.063		779		.327		39.30
1869	CD1			359		.507		577		301		37.82
1870		LEU				.787	44.			634		35.07
1871	С			359		.127		477		657		33.71
1872	0			359		.575		515		028		32.97
1873	N			360		.679		388		900		32.44
1874	CA			360		.646		105		610		31.57
1875	CB			360		.847		253		926		31.85
1876	CG1			360		.367		490		572		32.47
1877	CD1			360		.639		299		549		29.24
1878	CG2	ILE	А	360	-27	.934	41.	956	85.	801	1.00	30.72

# FIGURE 3AK

А	В	С	D	Ε	F	G	Н	I	J
1879	С	ILE	Α	360	-30.053	42.521	83.830	1.00	32.40
1880	0			360	-30.265	41.308	83.611		31.17
1881	N			361	-30.996	43.386	84.214	1.00	32.23
1882	CA			361	-32.363	42.958	84.445	1.00	34.85
1883	СВ			361	-33.223	44.060	85.087	1.00	35.23
1884	OG			361	-32.814	44.245	86.443	1.00	40.29
1885	C			361	-32.969	42.457	83.143	1.00	34.58
				361			83.147		
1886	O N				-33.734	41.528	82.017	1.00	34.46 35.27
1887		ARG			-32.571	43.020		1.00	
1888	CA			362	-33.116	42.553	80.736	1.00	35.84
1889	CB			362	-32.908	43.595	79.653	1.00	36.24
1890	CG	ARG			-33.797	44.805	79.768	1.00	
1891	CD	ARG			-33.312	46.000	78.930	1.00	48.93
1892	NE			362	-34.160	47.177	79.139	1.00	57.80
1893	CZ			362	-34.932	47.717	78.208	1.00	63.64
1894		ARG			-34.931	47.208	76.972	1.00	67.52
1895	NH2	ARG			-35.696	48.771	78.502	1.00	65.50
1896	С			362	-32.525	41.220	80.283	1.00	35.03
1897	0	ARG			-33.216	40.429	79.634	1.00	36.42
1898	N	LEU	Α	363	-31.279	40.939	80.664	1.00	32.41
1899	CA	LEU	Α	363	-30.645	39.705	80.279	1.00	32.03
1900	СВ	LEU	Α	363	-29.133	39.896	80.329	1.00	31.58
1901	CG	LEU	Α	363	-28.234	40.365	79.163	1.00	34.89
1902	CD1	LEU	Α	363	-28.757	40.467	77.803	1.00	36.09
1903	CD2	LEU	Α	363	-27.243	41.450	79.528	1.00	34.69
1904	С	LEU	Α	363	-31.027	38.572	81.203	1.00	32.15
1905	0	LEU	Α	363	-31.111	37.430	80.776	1.00	33.41
1906	N			364	-31.268	38.857	82.472	1.00	31.16
1907	CA			364	-31.571	37.770	83.428	1.00	32.01
1908	СВ			364	-30.963	38.067	84.804	1.00	31.60
1909	CG	LEU	Α	364	-29.420	38.146	84.738	1.00	31.16
1910	CD1	LEU			-28.840	38.468	86.102	1.00	34.77
1911	CD2	LEU			-28.841	36.783	84.213	1.00	
1912	C			364	-33.088	37.535	83.500	1.00	33.63
1913	0			364	-33.734	37.811	84.487	1.00	33.26
1914	N	LYS			-33.662	37.065	82.410	1.00	33.41
1915	CA	LYS			-35.082	36.796	82.393	1.00	35.64
1916	CB	LYS			-35.718				35.84
1917	CG			365	-35.929	38.880	81.125		39.34
1918	CD			365	-36.633	39.297	82.400		46.53
1919	CE				-37.698	40.335	82.107		49.18
				365					
1920	ΝZ			365	-37.064	41.556	81.577		54.14
1921	С			365	-35.216	35.299	82.375		35.57
1922	O			365	-34.516	34.626	81.599		34.77
1923	N			366	-36.084	34.780	83.241		34.63
1924	CA			366	-36.339	33.372	83.302		36.28
1925	CB			366	-37.437	33.047	84.346		35.81
1926	CG			366	-37.567	31.581	84.590		39.29
1927		HIS			-38.186	30.728	83.693		41.29
1928		HIS			-38.111	29.487	84.145		40.54
1929	NE2	HIS	А	366	-37.446	29.500	85.291	1.00	42.19

## FIGURE 3AL

A	В	С	D	E		F	G	Н	I	J
1930	CD2	HIS	Δ	366	_	37.088	30.796	85.587	1 00	39.35
1931	C			366		36.789	32.856	81.911	1.00	
1932	0			366		36.356	31.798	81.435	1.00	
1933	N			367		37.684	33.573	81.261	1.00	
				367		38.095		79.937		
1934	CA						33.069		1.00	
1935	CB	ASN				39.487	33.598	79.658	1.00	
1936	CG			367		40.080	33.074	78.380		44.28
1937	OD1			367		41.276	33.219	78.172		51.80
1938	ND2	ASN				39.271	32.476	77.525		46.36
1939	С	ASN				37.086	33.524	78.875	1.00	39.35
1940	0			367		36.961	34.709	78.683		38.80
1941	Ν			368		36.397	32.591	78.210	1.00	
1942	CA			368		35.336	32.903	77.238	1.00	
1943	СВ			368		34.976	31.536	76.624	1.00	
1944	CG	PRO	Α	368	_	35.451	30.502	77.567	1.00	40.15
1945	CD	PRO	Α	368	_	36.633	31.136	78.295	1.00	40.09
1946	С	PRO	Α	368	_	35.824	33.807	76.112	1.00	40.68
1947	0	PRO	Α	368	_	35.082	34.684	75.656	1.00	38.95
1948	N	SER	Α	369	_	37.064	33.592	75.664	1.00	42.38
1949	CA	SER	Α	369	_	37.639	34.437	74.597	1.00	43.99
1950	СВ	SER	Α	369	_	39.033	33.951	74.203	1.00	44.88
1951	OG	SER	Α	369		38.956	32.601	73.740	1.00	
1952	С			369		37.742	35.894	74.995		44.04
1953	0			369		37.889	36.754	74.140		44.29
1954	N			370		37.692	36.186	76.295		44.21
1955	CA			370		37.719	37.591	76.721		45.13
1956	СВ			370		38.437	37.739	78.053		45.55
1957	CG			370		39.839	37.121	77.994	1.00	
1958	CD			370		40.602	37.264	79.300	1.00	
1959	OE1	GLN				41.679	36.646	79.474	1.00	
1960	NE2	GLN				40.060	38.056	80.230	1.00	
1961	C			370		36.332	38.231	76.806		44.45
1962	0			370		36.210	39.423	77.063		44.24
1963	N	ARG				35.210	37.430	76.631		43.95
1964	CA	ARG		-						43.93
1965	CB	ARG				33.915	37.962 36.827	76.693		42.30
						32.911	36.206	76.882		
1966	CG	ARG				32.994		78.279	1.00	36.93
1967	CD	ARG				32.118		78.477		33.96
1968	NE	ARG				32.732	34.134	79.452		33.75
1969	CZ			371		32.561	32.828	79.521		32.13
1970		ARG				33.243	32.141	80.440		33.40
1971		ARG				31.717	32.197	78.702		30.58
1972	С	ARG				33.641	38.717	75.406		42.92
1973	0	ARG				34.115	38.306	74.374		43.48
1974	Ν			372		32.927	39.831	75.459		43.09
1975	CA			372		32.678	40.611	74.234		42.76
1976	СВ			372		31.890	41.837	74.717		43.00
1977	CG			372		31.590	41.648	76.178		42.62
1978	CD			372		32.371	40.456	76.678		43.28
1979	С			372		31.829	39.874	73.226		43.31
1980	0	PRO	Α	372	-	31.191	38.862	73.545	1.00	43.24

## FIGURE 3AM

А	В	С	D	Ε	F	G	Н	I	J
1981	N	MET	Α	373	-31.820	40.378	71.995	1.00	43.19
1982	CA			373	-30.928	39.857	70.976	1.00	43.50
1983	СВ	MET	Α	373	-31.448	40.174	69.585	1.00	44.61
1984	CG	MET		373	-32.688	39.421	69.205	1.00	50.78
1985	SD	MET		373	-33.173	39.941	67.576	1.00	64.15
1986	CE	MET		373	-32.985	41.823	67.726	1.00	59.77
1987	С	MET		373	-29.564	40.516	71.172	1.00	
1988	0	MET	Α	373	-29.452	41.539	71.841	1.00	39.32
1989	N	LEU	Α	374	-28.526	39.926	70.597	1.00	41.82
1990	CA	LEU	Α	374	-27.188	40.488	70.727	1.00	43.13
1991	СВ	LEU	Α	374	-26.194	39.605	70.025	1.00	43.22
1992	CG	LEU	Α	374	-25.814	38.411	70.923	1.00	45.40
1993	CD1	LEU	Α	374	-24.780	37.453	70.278	1.00	44.95
1994	CD2	LEU	Α	374	-25.284	38.861	72.288	1.00	41.96
1995	С	LEU	Α	374	-27.192	41.923	70.171	1.00	43.85
1996	0	LEU	Α	374	-26.478	42.788	70.667	1.00	
1997	N	ALA			-27.951	42.152	69.118	1.00	43.58
1998	CA	ALA			-27.979	43.472	68.494	1.00	44.11
1999	СВ	ALA			-29.028	43.491	67.388	1.00	
2000	С	ALA			-28.336	44.516	69.517		43.69
2001	0	ALA			-27.783	45.616	69.548	1.00	
2002	Ν	GLU			-29.265	44.123	70.370	1.00	43.44
2003	CA			376	-29.855	44.996	71.354	1.00	43.12
2004	CB			376	-31.147	44.357	71.836	1.00	43.67
2005	CG			376	-32.103	44.068	70.705	1.00	
2006	CD OF 1			376	-33.520	43.811	71.206	1.00	57.55
2007		GLU			-33.691	42.679 44.705	71.699	1.00	56.12
2008 2009	OE2 C	GLU		376	-34.454 -28.969	45.306	71.124 72.529	1.00	60.58 41.38
2010	0			376	-29.116	46.343	73.152	1.00	
2010	N	VAL			-28.059	44.394	72.850	1.00	39.33
2011	CA	VAL			-27.116	44.602	73.948	1.00	37.51
2013	CB	VAL			-26.405	43.276	74.328	1.00	36.63
2014		VAL			-25.281	43.536	75.284	1.00	35.55
2015	CG2				-27.416	42.254	74.883	1.00	37.26
2016	С	VAL			-26.043	45.547	73.449	1.00	37.40
2017	0	VAL	Α	377	-25.604	46.436	74.147	1.00	37.91
2018	N	LEU	А	378	-25.621		72.219		37.51
2019	CA			378	-24.580	46.115	71.589		39.81
2020	СВ	LEU	Α	378	-24.266	45.532	70.217	1.00	40.42
2021	CG	LEU	Α	378	-23.393	44.286	70.335	1.00	41.70
2022	CD1	LEU	Α	378	-23.067	43.658	68.983	1.00	46.77
2023	CD2	LEU	Α	378	-22.130	44.678	71.057		37.23
2024	С	LEU	Α	378	-24.946	47.580	71.442		41.32
2025	0			378	-24.075	48.445	71.358		42.45
2026	N	GLU			-26.244	47.845	71.421		41.71
2027	CA			379	-26.719	49.178	71.213		42.63
2028	СВ			379	-27.670	49.206	70.018		44.54
2029	CG			379	-26.995	48.791	68.724		47.20
2030	CD			379	-27.923	48.707	67.527		56.88
2031	OEI	GLU	А	379	-29.177	48.664	67.706	1.00	59.40

### FIGURE 3AN

А	В	С	D	E	F	G	Н	I	J
			_	0.00	0.000	10 665			
2032	OE2				-27.372	48.665	66.389		61.82
2033	С	GLU			-27.401	49.692	72.460	1.00	
2034	0	GLU			-28.071	50.749	72.435	1.00	
2035	N	HIS			-27.244	48.966	73.575	1.00	
2036	CA			380	-27.851	49.440	74.793		40.10
2037	СВ	HIS			-27.681	48.393	75.915		39.60
2038	CG	HIS			-28.332	48.789	77.191	1.00	
2039	ND1	HIS	Α	380	-29.551	48.279	77.590	1.00	40.40
2040	CE1	HIS	Α	380	-29.890	48.824	78.747	1.00	37.68
2041	NE2	HIS	Α	380	-28.923	49.643	79.122	1.00	39.48
2042	CD2	HIS	Α	380	-27.942	49.644	78.160		34.37
2043	С	HIS	Α	380	-27.163	50.747	75.172	1.00	39.36
2044	0	HIS	Α	380	-25.985	50.841	75.006	1.00	39.34
2045	N	PRO	Α	381	-27.882	51.732	75.713	1.00	40.21
2046	CA	PRO	Α	381	-27.277	53.041	75.975	1.00	40.19
2047	CB	PRO	Α	381	-28.439	53.885	76.518	1.00	40.84
2048	CG	PRO	Α	381	-29.677	53.167	76.093	1.00	42.96
2049	CD	PRO	Α	381	-29.307	51.702	76.106	1.00	40.74
2050	С	PRO	Α	381	-26.165	52.971	77.002	1.00	39.71
2051	0	PRO	Α	381	-25.239	53.739	76.860	1.00	38.49
2052	N	TRP	Α	382	-26.267	52.094	78.015	1.00	37.20
2053	CA	TRP	Α	382	-25.213	51.967	79.007	1.00	36.17
2054	CB	TRP	Α	382	-25.638	51.046	80.145	1.00	34.80
2055	CG	TRP	Α	382	-24.604	50.947	81.203	1.00	35.01
2056	CD1	TRP	Α	382	-24.349	51.852	82.170	1.00	36.17
2057	NE1	TRP	Α	382	-23.326	51.402	82.975	1.00	39.89
2058	CE2	TRP	Α	382	-22.895	50.191	82.505	1.00	36.83
2059	CD2	TRP	Α	382	-23.684	49.879	81.391	1.00	34.51
2060	CE3	TRP	Α	382	-23.437	48.680	80.716	1.00	37.27
2061	CZ3	TRP	Α	382	-22.450	47.843	81.185	1.00	35.85
2062	CH2	TRP	Α	382	-21.675	48.196	82.283	1.00	34.82
2063	CZ2	TRP		382	-21.887	49.357	82.966	1.00	32.53
2064	С	TRP		382	-23.940	51.436	78.346	1.00	36.25
2065	0	TRP		382	-22.833	51.887	78.657	1.00	36.89
2066	N	ILE			-24.090	50.456	77.472	1.00	36.03
2067	CA	ILE			-22.943	49.924	76.734	1.00	36.79
2068	СВ	ILE			-23.373	48.683	75.892	1.00	
2069	CG1				-23.751	47.476		1.00	34.61
2070	CD1	ILE	Α	383	-22.522	46.916	77.531		34.04
2071	CG2	ILE	Α	383	-22.221		75.038		35.05
2072	С	ILE			-22.377	51.014	75.804		39.31
2073	0	ILE			-21.172	51.250	75.708		40.13
2074	И	THR			-23.268	51.707	75.130		41.29
2075	CA	THR			-22.849	52.781	74.221		44.28
2076	СВ	THR			-24.120	53.418	73.673		44.01
2077	OG1	THR			-24.539	52.622	72.568		48.12
2078	CG2	THR			-23.822	54.750	73.090		49.09
2079	С	THR			-22.006	53.846	74.885		43.49
2080	0	THR			-20.980	54.271	74.359		46.02
2081	N	ALA			-22.449		76.044		42.28
2082	CA	ALA	Α	385	-21.779	55.332	76.763	1.00	42.24

### FIGURE 3AO

А	В	С	D	Ε	F	G	Н	I	J
2083	СВ			385	-22.705	55.884	77.823		41.95
2084	С			385	-20.509	54.897	77.424		42.41
2085	0			385	-19.606	55.728	77.660	1.00	
2086	Ν			386	-20.404	53.612	77.749		40.11
2087	CA			386	-19.254	53.178	78.478		38.95
2088	СВ			386	-19.696	52.453	79.740		
2089	CG			386	-20.371	53.392	80.739	1.00	
2090	OD1				-19.698	54.080	81.495	1.00	
2091		ASN			-21.695	53.396	80.754		40.56
2092	С			386	-18.195	52.366	77.760		
2093	0			386	-17.077	52.329	78.212		37.05
2094	Ν			387	-18.545	51.701	76.682	1.00	
2095	CA			387	-17.604	50.833	75.997	1.00	
2096	СВ			387	-18.322	49.922	75.010	1.00	
2097	OG			387	-17.359	49.075	74.356		42.67
2098	С			387	-16.573	51.578	75.172		43.18
2099	0			387	-16.930	52.538	74.482		43.25
2100	Ν			388	-15.344	51.059	75.181		44.22
2101	CA			388	-14.244	51.555	74.351	1.00	
2102	СВ			388	-12.908	51.070	74.888	1.00	
2103	OG			388	-12.725	51.591	76.195	1.00	
2104	С			388	-14.358	51.150	72.894	1.00	
2105	0			388	-15.115	50.231	72.549	1.00	
2106		ADP			-9.414	25.400	78.378		28.64
2107	PA			2001	-9.486	25.363	79.862		30.26
2108		ADP			-10.590	26.255	80.350	1.00	
2109		ADP			-9.587	23.880	80.555		30.98
2110	PB	ADP			-10.917	23.134	80.991		
2111		ADP			-11.692	24.139	81.826	1.00	
2112		ADP			-10.390	21.986	81.811	1.00	
2113		ADP			-11.688	22.740	79.755	1.00	
2114	05*			2001	-8.144	25.872	80.503	1.00	
2115	C5*	ADP			-8.004	25.866	81.924	1.00	
2116	C4*	ADP			-7.217	27.124	82.368		29.95
2117	04*	ADP			-5.951	27.178	81.679	1.00	
2118	C1*				-5.642	28.545	81.342	1.00	29.10
2119	C2*				-6.747	29.415	81.899		26.58
2120		ADP			-6.392	29.725	83.238		34.16
2121		ADP			-7.895	28.436	81.993		29.24
2122	03*			2001	-8.952	28.763	82.864		32.70
2123	N9			2001	-5.577	28.628	79.892		29.80
2124	C8			2001	-6.337	27.843	79.041		30.16
2125	N7			2001	-6.028	28.206	77.750		29.74
2126	C5			2001	-5.143	29.196	77.814		26.13
2127	C6	ADP			-4.519	29.877	76.813		29.08
2128	N6	ADP			-4.713	29.555	75.506		25.43
2129	C4			2001	-4.835	29.464	79.141		28.26
2130	N3			2001	-3.975	30.435	79.478		30.28
2131	C2 N1			2001	-3.350	31.144	78.490		31.73
2132	N1			2001	-3.633	30.829	77.180		29.64
2133	0	пОП	Λ.	3001	-9.988	28.798	79.067	T.00	31.10

## FIGURE 3AP

А	В	С	D	E	F	G	Н	I	J
2134	0	НОН	хз	003	-14.393	22.868	80.872	1.00	27.85
2135	0	HOH	Х3	004	-13.728	20.345	80.020	1.00	45.36
2136	0	HOH	Х3	005	-26.951	31.694	86.552	1.00	30.10
2137	0	НОН	Х3	006	-22.935	30.435	78.351	1.00	36.29
2138	0	НОН			-30.168	16.939	71.846		45.13
2139	0	НОН			-18.066	25.328	75.601	1.00	31.20
2140	0	НОН			-11.548	26.843	82.941	1.00	36.99
2141	0	НОН			-8.649	27.311	76.774	1.00	31.45
2142	0	НОН			-37.854	36.557	85.013	1.00	38.02
2143	0	НОН	Х3	012	-27.723	38.845	94.275	1.00	37.13
2144	0	НОН	Х3	013	-16.636	24.694	78.361	1.00	32.
2145	0	НОН	Х3	014	-8.241	35.027	68.248	1.00	33.00
2146	0	HOH	ХЗ	015	-0.912	17.916	82.933	1.00	36.14
2147	0	HOH	ХЗ	017	-15.066	34.944	89.120	1.00	42.99
2148	0	HOH	Х3	018	-22.824	25.783	92.176	1.00	46.76
2149	0	HOH	Х3	021	-11.944	23.669	84.418	1.00	39.47
2150	0	HOH	Х3	022	-12.703	21.499	77.561	1.00	40.61
2151	0	НОН	Х3	023	-37.367	42.995	79.960	1.00	59.45
2152	0	НОН	Х3	024	-5.576	15.379	86.195	1.00	66.48
2153	0	НОН	Х3	026	-8.353	43.652	79.479	1.00	44.84
2154	0	HOH	Х3	027	-23.236	19.714	67.938	1.00	47.17
2155	0	НОН	Х3	028	-10.809	32.568	66.377	1.00	35.26
2156	0	НОН	Х3	029	-15.673	31.938	88.442	1.00	44.34
2157	0	HOH	Х3	030	-0.223	35.059	71.257	1.00	55.88
2158	0	HOH	Х3	031	-20.254	50.297	89.242	1.00	49.49
2159	0	НОН			-4.408	26.185	61.520	1.00	57.94
2160	0	НОН			-6.464	20.470	80.244	1.00	42.32
2161	0	НОН			-26.908	54.727	81.094	1.00	46.09
2162	0	НОН			-3.500	31.862	81.803	1.00	
2163	0	НОН			-28.118	35.557	69.369	1.00	53.58
2164	0	НОН			-26.182	36.321	65.264	1.00	49.67
2165	0	НОН			14.155	34.581	65.299	1.00	48.35
2166	0	НОН			-34.861	43.555	76.702	1.00	53.19
2167	0	НОН			-39.173	35.975	82.307		45.97
2168	0	НОН			-14.153	39.758	92.741	1.00	38.14
2169	0	НОН			-17.759	51.104	95.196	1.00	
2170	0	НОН			-17.674	46.814	68.492	1.00	
2171	0	НОН			-21.016	27.883	83.182		40.34
2172	0	НОН			-32.376	28.743	75.835		35.07
2173	0	НОН			-26.582	54.610	84.614		51.10
2174	0	НОН			-28.989	37.779	69.028		45.59
2175	0	НОН			1.044	35.132	80.541		40.83
2176	0	НОН			-18.143	48.279	89.631		35.13
2177 2178	0	HOH HOH			-22.772 -28.242	50.169 40.105	87.633		35.90 39.46
2178	0	НОН			-28.242 -5.648	27.887	67.233 86.644		45.28
21/9	0	НОН			-22.278	29.579	81.107		46.99
2180	0	НОН			-21.804	27.943	85.859	1.00	31.17
2182	0	НОН			-19.327	55.542	84.158		69.06
2183	0	НОН			-16.658	53.812	86.138	1.00	76.39
2184	0	НОН			-11.616	48.407	86.048		44.96
2101	J	11011	-10	550	11.010	10.107	00.010	±•00	11.70

# FIGURE 3AQ

A	В	С	D	E	F	G	Н	I	J
0105	_			0.61	25 202	41 264	70 456	1 00	40.60
2185	0	НОН			-35.280	41.364	78.456		43.63
2186	0	НОН			-35.848	29.209	81.326	1.00	50.09
2187	0	НОН			-20.386	19.911	74.001	1.00	46.93
2188	0	НОН			-5.444	37.823	84.054	1.00	35.84
2189	0	НОН			-2.738	38.173	71.721	1.00	
2190	0	НОН			-3.973	35.760	72.248	1.00	33.90
2191	0	HOH			-29.746	39.136	96.635	1.00	62.80
2192	0	HOH			-14.064	25.472	82.227	1.00	31.69
2193	0	HOH	Х2	089	-4.484	33.261	84.056	1.00	47.20
2194	0	НОН	Х2	090	-9.895	27.055	74.329	1.00	27.24
2195	0	HOH	Х2	091	-0.170	31.678	70.061	1.00	29.25
2196	0	HOH	Х2	092	-1.106	31.853	83.735	1.00	53.32
2197	0	HOH	Х2	093	-25.264	41.053	66.798	1.00	59.10
2198	0	HOH	X2	094	-25.466	43.888	65.479	1.00	69.73
2199	0	НОН	Х2	095	-32.272	31.292	69.214	1.00	67.50
2200	0	HOH	Х2	096	-24.385	33.367	89.916	1.00	31.89
2201	0	HOH	Х2	097	-14.677	21.587	82.263	1.00	41.33
2202	0	HOH	Х2	098	-15.335	22.257	78.530	1.00	36.43
2203	0	HOH	Х2	099	-11.146	29.804	67.165	1.00	47.94
2204	0	HOH	Х2	100	-9.610	28.214	65.560	1.00	46.43
2205	MG	MG	Х2	086	-13.528	22.597	79.198	1.00	12.09
2206	MG	MG	Х2	088	-12.337	25.921	81.074	1.00	12.20
2207	P	PO4	Х2	002	-24.838	17.852	76.312	1.00	54.63
2208	01	PO4	X2	002	-24.694	18.499	74.963	1.00	59.50
2209	02	PO4	Х2	002	-26.204	17.207	76.361	1.00	64.72
2210	03	PO4	Х2	002	-23.779	16.793	76.532	1.00	57.00
2211	04	PO4	Х2	002	-24.798	18.859	77.420	1.00	60.01